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

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Overview of Invited Talks and Sessions
(Lecture halls H43, H44, H45, and H46; Poster C)

Invited Talks

MM 1.1	Mon	9:30–10:00	H43	**Salient features of phase stability and mechanical properties of high-entropy alloys** — •Easo George
MM 7.1	Mon	15:00–15:30	H43	**Thermodynamics and optical response of nanoscale systems from atomistic simulations** — •Paul Erhart, Tuomas Rossi, Magnus Rahm, Mikael Kuisma
MM 13.1	Tue	9:30–10:00	H43	**Single Nanoparticle Insights to Create the Fastest Hydrogen Sensor in the World** — •Christoph Langhammer
MM 21.1	Wed	9:30–10:00	H43	**Rational design of Cu based shape memory alloys with low functional fatigue properties** — •Xian Chen, Mostafa Karami
MM 30.1	Wed	18:15–18:45	H43	**Advanced *in situ* Electron Microscopy for targeted Battery Development** — •Benjamin Butz
MM 32.1	Thu	9:30–10:00	H43	**The Digital Transformation in Materials Science and Solid State Physics** — •Chris Eberl et al.

Invited talks of the joint Symposium SKM Dissertation-Prize 2019
See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30– 9:50	H2	**Synchronization and Waves in Confined Complex Active Media** — •Jan Frederik Totz
SYSD 1.2	Mon	9:50–10:10	H2	**Spin scattering of topologically protected electrons at defects** — •Philipp Rüssmann
SYSD 1.3	Mon	10:10–10:30	H2	**Beyond the molecular movie: Revealing the microscopic processes behind photo-induced phase transitions** — •Chris W. Nicholson
SYSD 1.4	Mon	10:30–10:50	H2	**Thermodynamic bounds on current fluctuations** — •Patrick Pietzonka
SYSD 1.5	Mon	10:50–11:10	H2	**Lightwave-driven quasiparticle acceleration** — •Fabian Langer
SYSD 1.6	Mon	11:10–11:30	H2	**Ultrafast plasmon-driven point-projection electron microscopy** — •Jan Vogelsang
SYSD 1.7	Mon	11:30–11:50	H2	**Helimagnets, sand patterns and fingerprints linked by topology** — •Peggy Schönherr

Invited talks of the joint Symposium Mechanically Controlled Electrical Conductivity of Oxides
See SYCO for the full program of the symposium.

SYCO 1.1	Mon	9:30–10:00	H1	**Dislocation Dynamics and Their Conductivities in Oxides** — •Yuichi Ikuhara
SYCO 1.2	Mon	10:00–10:30	H1	**Strain effects in ionic conductivity and electrode processes** — •Jürgen Janek
SYCO 1.3	Mon	10:30–11:00	H1	**Elastic dipoles of point defects in materials** — •Celine Varvenne
SYCO 1.4	Mon	11:30–12:00	H1	**Mapping strain/pressure with ZnO nanowire arrays by piezo-phototronic effect** — •Caofeng Pan

SYCO 1.5   Mon   12:00–12:30   H1   **Bulk and Flexo-photovoltaic effect** — •Marin Alexe

Invited talks of the joint Symposium Czech Republic as Guest of Honor
See SYCZ for the full program of the symposium.

SYCZ 1.1	Thu	9:30–10:00	H4	**Crystal symmetries and transport phenomena in antiferromagnets** — •Tomas Jungwirth
SYCZ 1.2	Thu	10:00–10:30	H4	**Terahertz subcycle charge and spin control** — •Rupert Huber
SYCZ 1.3	Thu	10:30–11:00	H4	**1D molecular system on surfaces** — •Pavel Jelinek
SYCZ 1.4	Thu	11:15–11:45	H4	**Tunneling microscopy on insulators provides access to out-of-equilibrium charge states** — •Jascha Repp
SYCZ 1.5	Thu	11:45–12:15	H4	**Occam's razor and complex networks from brain to climate** — •Jaroslav Hlinka
SYCZ 1.6	Thu	12:15–12:45	H4	**Long range temporal correlations in complex systems** — •Holger Kantz

Invited talks of the joint Symposium Physics of Self-Organization in DNA Nanostructures
See SYDN for the full program of the symposium.

SYDN 1.1	Thu	9:30–10:00	H1	**Functional DNA Nanostructures and Their Applications** — •Itamar Willner
SYDN 1.2	Thu	10:00–10:30	H1	**Gaining control of DNA-based nanodevices** — •Francesco Ricci
SYDN 1.3	Thu	10:30–11:00	H1	**Self-assembly and optical properties of single molecule polymers on DNA origami** — •Kurt Gothelf
SYDN 1.4	Thu	11:15–11:45	H1	**DNA origami route to dynamic plasmonics** — •Laura Liu
SYDN 1.5	Thu	11:45–12:15	H1	**DNA templated metal nanostructures** — •Ralf Seidel

Sessions

MM 1.1–1.1	Mon	9:30–10:00	H43	**Invited talk George**
MM 2.1–2.9	Mon	10:15–13:15	H43	**Topical session (Symposium MM): High entropy and compositionally complex alloys**
MM 3.1–3.5	Mon	10:15–11:30	H44	**Materials for Energy Storage and Conversion**
MM 4.1–4.11	Mon	10:15–13:15	H45	**Methods in Computational Materials Modelling (methodological aspects, numerics)**
MM 5.1–5.10	Mon	10:15–13:00	H46	**Mechanical Properties**
MM 6.1–6.5	Mon	11:45–13:15	H44	**Topical session (Symposium MM): Correlative and in-situ Microscopy in Materials Research**
MM 7.1–7.1	Mon	15:00–15:30	H43	**Invited talk Erhart**
MM 8.1–8.7	Mon	15:45–18:30	H43	**Topical session (Symposium MM): High entropy and compositionally complex alloys**
MM 9.1–9.10	Mon	15:45–19:00	H44	**Topical session (Symposium MM): Correlative and in-situ Microscopy in Materials Research**
MM 10.1–10.11	Mon	15:45–18:45	H45	**Methods in Computational Materials Modelling (methodological aspects, numerics)**
MM 11.1–11.7	Mon	15:45–18:30	H46	**Symposium SYCO of the divisions MM (leading), O, CPP, KFM and DS continued as topical session: Mechanically controlled electrical conductivity of oxides (joint session MM/CPP/O)**
MM 12.1–12.37	Mon	19:15–20:45	Poster C	**Poster session I**
MM 13.1–13.1	Tue	9:30–10:00	H43	**Invited talk Langhammer**
MM 14.1–14.9	Tue	10:15–13:15	H43	**Topical session (Symposium MM): High entropy and compositionally complex alloys**
MM 15.1–15.8	Tue	10:15–13:15	H44	**Topical session (Symposium MM): Correlative and in-situ Microscopy in Materials Research**
MM 16.1–16.11	Tue	10:15–13:15	H45	**Methods in Computational Materials Modelling (methodological aspects, numerics)**
MM 17.1–17.10	Tue	10:15–13:00	H46	**Nanomaterials**

MM 18.1–18.5	Tue	14:15–15:30	H45	**Interfaces**
MM 19.1–19.6	Tue	14:15–15:45	H46	**Miscellaneous: Biomaterials, Magnetic Shape Memory Alloys, Sensors and Actuators (joint session MM/MA)**
MM 20.1–20.36	Tue	18:30–20:00	Poster C	**Poster session II**
MM 21.1–21.1	Wed	9:30–10:00	H43	**Invited talk Chen**
MM 22.1–22.11	Wed	10:15–13:15	H43	**Materials for Energy Storage and Conversion**
MM 23.1–23.11	Wed	10:15–13:15	H44	**Methods in Computational Materials Modelling (methodological aspects, numerics)**
MM 24.1–24.9	Wed	10:15–13:15	H45	**Topical session (Symposium MM): Correlative and in-situ Microscopy in Materials Research**
MM 25.1–25.11	Wed	10:15–13:15	H46	**Transport (Diffusion, conductivity, heat)**
MM 26.1–26.12	Wed	15:00–18:15	H43	**Materials for Energy Storage and Conversion**
MM 27.1–27.12	Wed	15:00–18:15	H44	**Methods in Computational Materials Modelling (methodological aspects, numerics)**
MM 28.1–28.7	Wed	15:00–17:45	H45	**Topical session (Symposium MM): Correlative and in-situ Microscopy in Materials Research**
MM 29.1–29.12	Wed	15:00–18:15	H46	**Microstructure and Phase Transformations**
MM 30.1–30.1	Wed	18:15–18:45	H43	**Invited talk Butz**
MM 31	Wed	19:00–20:00	H43	**General Meeting of the Metal- and Materials Division and Best Poster Award**
MM 32.1–32.1	Thu	9:30–10:00	H43	**Invited talk Eberl**
MM 33.1–33.9	Thu	10:15–13:15	H43	**Topical session (Symposium MM): Big Data Analytics in Materials Science**
MM 34.1–34.10	Thu	10:15–13:00	H44	**Methods in Computational Materials Modelling (methodological aspects, numerics)**
MM 35.1–35.7	Thu	10:15–13:00	H45	**Topical session (Symposium MM): Correlative and in-situ Microscopy in Materials Research**
MM 36.1–36.10	Thu	10:15–13:00	H46	**Liquid and Amorphous Metals**
MM 37.1–37.11	Thu	15:00–18:45	H43	**Topical session (Symposium MM): Big Data Analytics in Materials Science**
MM 38.1–38.9	Thu	15:00–17:30	H44	**Methods in Computational Materials Modelling (methodological aspects, numerics)**
MM 39.1–39.8	Thu	15:00–17:45	H45	**Structural Materials (Steels, light-weight materials, high-temperature materials)**
MM 40.1–40.5	Thu	15:00–16:15	H46	**Liquid and Amorphous Metals**

Annual General Meeting of the Metal and Material Physics Division

Wednesday   19:00–20:00   H43

MM 1: Invited talk George

Time: Monday 9:30–10:00   Location: H43

Invited Talk   MM 1.1   Mon 9:30   H43
Salient features of phase stability and mechanical properties of high-entropy alloys — •Easo George — Oak Ridge National Laboratory, Oak Ridge, TN, USA

High-entropy alloys (HEAs) are a relatively new class of materials and are of interest because of their potential for useful properties: for example, high strength combined with high ductility and toughness. In this talk, I will review recent progress in understanding phase stability and mechanical properties of face-centered cubic (FCC) HEAs. Phase stability is important because it can have both beneficial and harmful effects on strength and ductility. Decomposition of an ini-

tially single-phase FCC alloy into intermetallic phases causes severe embrittlement whereas a polymorphic FCC to HCP transformation enhances work hardening rate and ductility. The latter involves twinning and/or transformation induced plasticity, both of which correlate with low stacking fault energy. To the extent possible I will explain macroscopic aspects of flow and fracture in terms of salient microscopic features such as dislocation structures, stacking faults, twins and their evolution with strain, temperature and chemical composition. Research supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

MM 2: Topical session (Symposium MM): High entropy and compositionally complex alloys

Sessions: Design and Development; Properties I

Time: Monday 10:15–13:15   Location: H43

Topical Talk   MM 2.1   Mon 10:15   H43
Fundamentals of deformation in high- and medium-entropy alloys — •Guillaume Laplanche[1], Joël Bonneville[2], Céline Varvenne[3], Aleksander Kostka[4], William A. Curtin[5], and Easo P. George[6] — [1]Institut für Werkstoffe, Ruhr-Universität Bochum, Germany — [2]Institut PPRIME, University of Poitiers, France — [3]CINaM, Aix-Marseille Univ. - CNRS, Marseille, France — [4]Materials Research Department and Center for Interface Dominated Materials (ZGH), Ruhr-University Bochum, Germany — [5]Institute of Mechanical Engineering, EPFL, Lausanne, Switzerland — [6]Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, USA

High-entropy alloys (HEAs) consists of five or more elements in near-equiatomic proportions and crystallize as single-phase solid solutions. This presentation focuses on one of the most thoroughly investigated HEAs, namely, the fcc CrMnFeCoNi alloys. These alloys have been shown to exhibit fascinating mechanical properties, including increasing tensile ductility and strength with decreasing temperature, with composition having a strong effect. In this presentation, two model alloys: CrMnFeCoNi (HEA) and CrCoNi (medium-entropy alloy), are selected to explain key microstructural aspects responsible for strength, ductility, and work-hardening rate. As both alloys deform by dislocation plasticity initially and deformation twinning after a critical stress has been reached, evolutions with deformation of dislocation and twin microstructures as well as activation volumes are used to identify the mechanisms responsible for macroscopic mechanical behaviors.

Development of New Compositionally Complex Alloys for Laser Additive Manufacturing — •Fabian Kies[1], Simon Ewald[2], Bengt Hallstedt[3], and Christian Haase[1] — [1]IEHK Steel Institute, 52072 Aachen, Germany — [2]Digital Additive Production DAP, 52074 Aachen, Germany — [3]Materials Applications in Mechanical Engineering IWM, 52072 Aachen, Germany

MM 2.2   Mon 10:45   H43

Exploring the field of compositionally complex alloys (CCAs) by capitalizing on the flexibility of additive manufacturing (AM) provides the opportunity to design new metals with exceptional mechanical properties. So far, efficient CCA development is held up by time-consuming manufacturing methods. Therefore, a methodology is introduced which enables flexible exploration and design of CCAs by combining theoretical and experimental approaches, thereby focusing on the Al-C-Co-Cr-Fe-Mn-Ni alloying system. A self-compiled thermodynamic database for CALPHAD was used to identify promising composition ranges for the system, which were subsequently synthesized using elemental powder blends in AM processes. Materials characterization was split into light (XRD, hardness) and deep (SEM, EBSD, tensile test) screening to increase characterization speed. Precipitate types in the manufactured samples were correctly predicted by the theoretical screening. Properties identified by light screening steps translated reliably into the deep screening stage. The applicability of the introduced methodology to identify promising CCAs well as the resulting microstructural and mechanical properties in the Al-C-Co-

Cr-Fe-Mn-Ni alloying system are discussed.

MM 2.3   Mon 11:00   H43
Electrodeposition of high entropy alloy thin films and nanowires — •Mirko Gabski, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Münster, Germany

High-entropy alloys consisting of four of more elements in nearly equiatomic concentrations have attracted attention as structural materials due to their favorable physical and mechanical properties, especially at elevated temperatures as well as improved corrosion and oxidation resistance when compared to more common alloys. The aforementioned properties make high-entropy alloy an interesting choice as a material for the coating of metal parts. In this work electrodeposition is used to obtain thin films of an AlCoCrFeNi alloy to investigate the influence of the deposition conditions on its composition and morphology using energy disperse X-ray spectroscopy and scanning electron microscopy. Furthermore the fabrication of nanowires is carried out utilizing nanostructured anodic aluminum oxide as a template to investigate the influence of the nano-confinement on the deposition process and the resulting microstructure.

MM 2.4   Mon 11:15   H43
Nanoscale, continuous phase separation of Al-containing compositionally complex alloys via Laser Powder Bed Fusion — Nicolas J. Peter[1], •Hyo Yun Jung[1], Eric Gärtner[2], Volker Uhlenwinkel[2], Gerhard Dehm[1], and Eric A. Jägle[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Leibniz IWT, Bremen, Germany

Literature shows that increasing Al-additions to the Cantor alloy transformed the initially single-phase FCC (A1) alloy to a BCC (A2 matrix/B2 precipitates) material with superior strength in casts. In contrast to such previous studies, we make use of the selective laser melting process. We investigate three different compositionally complex alloys, namely AlCoCrFeNi, AlMnCoCrFeNi and AlCu$_{0.5}$FeNiCoCr$_{0.75}$. The same microstructure is found for all three alloys using advanced electron microscopy consisting of a coherent two-phase structure with interwoven A2/B2 phases. Atom probe tomography confirms the nanoscale phase separation into Ni-Al and Fe-Cr domains. An effect of the intrinsic heat treatment can be excluded as the gas atomized powder used for selective melting already contained both phases. In addition, melt spun reference samples of AlCu$_{0.5}$FeNiCoCr$_{0.75}$ were investigated and found to adopt the same interwoven A2/B2 microstructure. Our results therefore point to a conditional spinodal decomposition process, which is currently further investigated. Finally, first results on establishing the structure-property relationships are presented.

15 min. break

Topical Talk   MM 2.5   Mon 11:45   H43
Single-crystal mechanical properties of equiatomic CrMnFeCoNi high-entropy alloy and its derivative equiatomic quater-

nary and ternary medium-entropy alloys — •Haruyuki Inui — Department of Materials Science and Engineering, Kyoto University, Kyoto, Jpan

The plastic deformation behavior of single crystals of the FCC equatomic CrMnFeCoNi high-entropy alloy and its derivative quaternary (CrFeCoNi) and ternary (CrCoNi) medium-entropy alloys has been investigated in a temperature range of 10-1273 K. Deformation occurs via slip of the {111}<110> system exclusively in the whole temperature range for all alloys investigated. The CRSS values increase with decreasing temperature, especially below room temperature, so that the concept of *stress equivalence* is obeyed for all alloys investigated. This is a clear indication that the strength of these alloys should be described by a mechanism based on solid-solution hardening. The CRSS values at 10 K seems to be well scaled with the mean-square atomic displacement from the regular FCC lattice points (calculated based on density-functional theory). Dislocations are observed to dissociate widely into Shockley partials for all alloys investigated, indicating their low stacking fault energies (below 30 mJ/m2). Deformation twinning occurs in later stages of deformation at low temperatures below room temperature in many of these alloys. The correlation between twinning stress and the stacking-fault energy will be discussed.

MM 2.6   Mon 12:15   H43
High-pressure torsion produced lamellar structure between single phaseequiatomic FCC CoCrFeMnNi and single phase BCC HfNbTaTiZr HEAs — •Shabnam Taheriniya, Sergiy V. Divinski, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Münster, Germany

High-pressure torsion (HPT) was utilized to analyze deformation induced bonding and mixing of dissimilar high entropy alloys (HEAs). A single phase equiatomic FCC Cantor alloy, CoCrFeMnNi, and equiatomic HfNbTaTiZr as a single phase BCC HEA are attached and deformed for 5, 10 and 15 revolutions using HPT with a pressure of 9 GPa. The resulting structure and the local microstructure at the interfaces are observed and analyzed using scanning electron microscopy (SEM), electron back-scatter diffraction (EBSD) and transmission electron microscopy (TEM). Furthermore, the chemical composition at the interface is investigated using energy dispersive X-ray spectroscopy (EDX). The results are discussed and analyzed with respect of the mechanisms responsible for shear induced mixing/bonding at the interfaces under the specific conditions provided by high entropy alloys.

MM 2.7   Mon 12:30   H43
Tunable optical properties of (Mg-Co-Cu-Ni-Zn)O High Entropy Oxide thin films — •Emeline Michel — I. Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany

Multi-component High Entropy Alloys have been shown to be interesting for their favorable mechanical properties, e.g. high fracture toughness, and resistance to oxidizing or corrosive environment. The enhanced properties of High Entropy Alloys are due to the entropy-driven formation of simple phases. However, the oxidation of these materials, leading to High Entropy Oxides, is poorly understood. High Entropy Oxides have been recently studied by Rost et al., who verified the entropy stabilization ansatz and showed that configurational disorder provides an alternative route to new materials discovery.

Here we investigate the oxidation behaviour of High Entropy Alloys from the Mg-Co-Cu-Ni-Zn metallic system. Therefore, thin films of High Entropy Oxides are deposited by reactive sputtering. Sur-

prisingly, we observe that the system exhibits a pronounced, broad sub-bandgap absorption. Moreover, the oxygen partial pressure used to deposit the (Mg-Co-Cu-Ni-Zn)O thin films is a tuning parameter of the optical properties of the system. The correlation between the tunable optical properties of (Mg-Co-Cu-Ni-Zn)O thin films and its structural changes is investigated.

MM 2.8   Mon 12:45   H43
The effect of magnetism on the stability of high entropy alloys — •Jakub Šebesta[1,2] and Dominik Legut[1] — [1]IT4Innovation, VŠB-TU Ostrava, 17.listopadu 15, 708 33 Ostrava-Poruba, Czech Republic — [2]Charles University, Faculty of Mathematics and Physics, Department of Condensed Matter Physics, Ke Karlovu 5, 121 16 Praha 2, Czech Republic

Multi-principal elements alloys, called as 'High Entropy Alloys', represent a promising group of materials, due to its possible applications in the industry. They form a single phase solid solution based on high number of components in near-equimolar composition, that often brings a high entropy contribution to the Gibbs free energy. It is considered as the main contribution stabilizing the alloy at higher temperatures. In the current work we'd like to focus on another contributions, which could affect stability of the system, i.e magnetic interactions among all atoms. Using ab-initio calculations based on TB-LMTO-ASA within CPA we studied the stability of the well known 'Cantor alloy' CoCrFeMnNi as well as related phases with a nonmagnetic substitution were calculated. For a similar reason non-homogeneous structures and magnetic exchange interactions were studied as well. We show strenghts of the mutual interactions between the elements and their impacts on the stability of the alloy. Further we discuss the importance and its contribution of mutual exchange ineraction to the final preferred magnetic ordering of studied phase. Finally we'll suggest possible way for stabilizing the parent structure.

MM 2.9   Mon 13:00   H43
On the mechanism of displacive phase transformation in metastable high entropy alloys — •Jing Su, Dierk Raabe, and Zhiming Li — Max-Planck-Institut für Eisenforschung GmbH, Dusseldorf, Germany

High-entropy alloys (HEAs) have drawn increasing attention in the past decade due to their massive solid-solution compositional space and promising mechanical properties. Recently, non-equiatomic metastable HEAs with tunable stacking fault energy have shown improved mechanical properties with an even larger compositional freedom and a broader range for microstructure design compared to the equiatomic stable HEAs. This is related to the joint activation of multiple deformation mechanisms including transformation induced plasticity (TRIP) and/or twinning induced plasticity (TWIP). In the current study, a metastable interstitial carbon-doped HEA (iHEA) has been chosen and subjected to cold rolling. Interestingly, deformation-driven forward and reverse (bidirectional) martensitic transformation has been observed in the current iHEA with a well-tuned stacking fault energy. The mechanisms of such bidirectional displacive transformation and the associated nanostructure formation have been investigated by electron channeling contrast imaging (ECCI), electron backscattered diffraction (EBSD) and high-resolution transmission electron microscopy (HR-TEM). We also discuss the mechanical properties of the nanostructured specimens and the corresponding work hardening behavior to shed light on the design of strong and ductile bulk nanostructured HEAs via displacive transformation.

MM 3: Materials for Energy Storage and Conversion

New Battery Materials

Time: Monday 10:15–11:30   Location: H44

MM 3.1   Mon 10:15   H44

Li3OCl thin film as a solid state electrolyte — ●Kun Zhang, Efi Hadjixenophontos, Yug Joshi, and Guido Schmitz — Chair of Materials Physics, Institute of Materials Science, University of Stuttgart, Heisenberg Straße 3, 705969 GERMANY

In comparison with conventional batteries, solid state batteries offer safety and higher energy density. In this work, Li-rich Li3OCl is studied as a potential solid-state electrolyte in Li-Ion batteries. Thin Li3OCl films (50~200 nm) are deposited by applying a composite target (Li2CO3+LiCl) via Ion Beam Sputtering. The composition of the films is investigated by XRD and XPS, and the thickness is evaluated by FIB cross-sections. The ionic and the electrical conductivity are determined using Pt/Li3OCl/Pt structure by Electrochemical Impedance Spectroscopy and *10-7 S/cm and *10-11 S/cm are achieved respectively at 25 °C. Furthermore, the activation energy of Li3OCl is derived from the measured ionic conductivity from 25 °C up to 140 °C and is equal to 0.57 eV.

MM 3.2   Mon 10:30   H44

Controlling oxygen defects in $Li_4Ti_5O_{12}$ (LTO) — ●C. Grosu[1,2], P. Jakes[1], T. Gigl[2], C. Hugenschmidt[2], D. Haering[2], J. Granwehr[1], R.A. Eichel[1], K. Reuter[2], and C. Scheurer[2] — [1]IEK-9, FZ Jülich — [2]TU München

Spinel $Li_4Ti_5O_{12}$ (LTO) is an interesting anode material for next-generation all solid state Li-ion batteries (ASSB). Its "zero strain" charge/discharge behavior promises high safety and long cycling lifetimes. Yet, pristine, white LTO possesses poor ionic and electronic conductivity. The latter can be increased by tailoring the sintering protocol to produce oxygen vacancies, resulting in a performing, blue LTO material. Hitherto, the detailed structure and distribution of the vacancies is not known. Producing a controlled gradient of vacancies will help understanding, first what the fundamental impact on the conductivity is and later optimizing the design of the material itself. We will discuss a controlled procedure to introduce oxygen vacancies, creating a gradient of defects from the surface to bulk. In a combined experimental and theoretical approach, the resulting disordered, defect-rich LTO structures are analyzed and theoretical defect models compared to the results of depth-resolved positron coincidence Doppler broadening spectroscopy (CDBS) measured at the Garching positron source NEPOMUC.

MM 3.3   Mon 10:45   H44

Weberite-type sodium metal fluorides - promising cathode materials for sodium ion batteries — ●Holger Euchner[1], Anji Reddy[1], Oliver Clemens[2], and Gross Axel[1,3] — [1]Helmholtz Institute for Electrochemical Energy Storage, Ulm, Germany — [2]Materials Design by Synthesis, Technical University Darmstadt, Darmstad, Germany — [3]Institute of Theoretical Chemistry, Ulm University, Ulm, Germany

Among alternative battery technologies suggested for substituting the state of the art lithium-ion batteries (LIBs) Na ion batteries (NIBs) are one of the most promising candidates. However, due to the lower operating potential of the cathode material in current NIBs their specific energy is significantly lower than in LIBs. To compete with the high energy density of LIBs, high voltage cathode materials are required for NIBs. Here, we report a computational investigation of weberite-type sodium metal fluorides ($Na_2MM'F_7$), a new class of so far unexplored high voltage and high energy density materials. A series of known and hypothetical compounds with weberite-type structure are investigated and their potential as cathode materials for NIBs is evaluated. Weberite-type $Na_2MM'F_7$ shows quasi-three-dimensional Na diffusion with surprisingly low activation barriers. The high energy density combined with low barriers for Na diffusion makes $Na_2MM'F_7$ type compounds promising candidates for cathode materials in NIBs.

MM 3.4   Mon 11:00   H44

Highly nitrogen doped carbon nanofibers with superior rate capability and cyclability for potassium ion batteries — ●Chenglin Zhang, Yang Xu, Long Liu, and Yong Lei — Institute für Physics & IMN MacroNano (ZIK), Technische Universität Ilmenau, Ilmenau 98693, Germany

Potassium-ion batteries are a promising alternative to lithium-ion batteries. However, it is challenging to achieve fast charging/discharging and long cycle life with the current electrode materials because of the sluggish potassiation kinetics. Here, we report a soft carbon anode, namely highly nitrogen-doped carbon nanofibers, with superior rate capability and cyclability. Quantitative analysis and theoretical simulations were employed to interpret the benefits of nitrogen doping and demonstrate the advantage of the pyrrolic and pyridinic N dopants over the quaternary N dopant. Surface-dominated K-storage is verified by quantitative kinetics analysis and theoretical investigation.[1] Considering the cost-effectiveness and material sustainability, our work may shed some light on searching for K-storage materials with high performance.

[1] Yang Xu; Chenglin Zhang; Min Zhou; Qun Fu; Chengxi Zhao; Minghong Wu* and Yong Lei*[J] Nature Commun. (2018) 9:1720.

MM 3.5   Mon 11:15   H44

2D/3D Organo-metal Hybrid Perovskite Photobatteries — ●Angus Mathieson, Felix Deschler, and Michael DeVolder — University of Cambridge, Cambridge, United Kingdom

Increases in the global energy demand necessitate the development of new approaches to energy conversion and storage. In particular, the utilisation of solar energy could provide a basis of evolving technologies capable of meeting modern demands.

By combining the photovoltaic and newfound electrochemical properties of organo-metal hybrid perovskite materials in a single device, a novel photobattery technology is proposed. Utilising the photovoltaic performance of bulk 3D perovskite materials in combination with the intercalation and conversion mechanisms available to Lithium ion species of layered 2D perovskite materials, a device with the ability both to convert light to electrochemical energy and store it is discussed. The motivation for such a device will be demonstrated, with its inherent impact in areas such as off-grid energy solutions and the internet of things. The fabrication techniques are described and characterisation techniques common to both photovoltaic and electrochemical disciplines, with their recent results are discussed. The current understanding of the charge carrier dynamics and device structure under electrochemical cycling are discussed in depth followed by recent developments in device performance and characterisation. Given the potential commercial applicability of the device, ideas to enhance the device performance whilst reducing fabrication cost and increasing scale are used in conclusion.

MM 4: Methods in Computational Materials Modelling (methodological aspects, numerics)

Sessions: Automated workflows and High throughput searches

Time: Monday 10:15–13:15 Location: H45

MM 4.1 Mon 10:15 H45

Formation enthalpies for automated computational materials design — •Rico Friedrich[1], Demet Usanmaz[1], Corey Oses[1], Andrew Supka[2], Marco Fornari[2], Marco Buongiorno Nardelli[3], Cormac Toher[1], and Stefano Curtarolo[4] — [1]Dept. of Mech. Eng. and Mat. Sci., Duke Univ. — [2]Dept. of Phys. and Science of Advanced Materials Program, Central Michigan Univ. — [3]Dept. of Phys. and Dept. of Chem., Univ. of North Texas — [4]Mat. Sci., Elec. Eng., Phys. and Chem., Duke Univ.

The accurate calculation of formation enthalpies is crucial for computational materials design. For compounds chemically similar to their reference phases such as metal alloys, standard semi-local approximations to density functional theory (DFT) lead to accurate results [1]. When the phases are chemically dissimilar as in the case of oxides, DFT suffers from a lack of error cancellation leading to deviations of several hundred meV/atom compared to experimental values [2]. We use the automated computational materials design framework AFLOW [3] to validate correction schemes for *ab-initio* formation enthalpies [2, 4]. These empirical methods can improve DFT predictions by a factor of 4 to 7. Zero-point vibrational and thermal contributions to the formation enthalpy are found to largely cancel each other.
[1] S. Curtarolo *et al.*, Calphad **29**, 163-211 (2005).
[2] V. Stevanović *et al.*, Phys. Rev. B **85**, 115104 (2012).
[3] S. Curtarolo *et al.*, Comput. Mater. Sci. **58**, 218 (2012).
[4] L. Wang *et al.*, Phys. Rev. B **73**, 195107 (2006).

MM 4.2 Mon 10:30 H45

Accelerating high-throughput searches for new alloys with active learning of interatomic potentials — •Konstantin Gubaev[1], Evgeny Podryabinkin[1], Gus Hart[2], and Alexander Shapeev[1] — [1]Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Nobel str. 3, Moscow 143026, Russia — [2]Department of Physics and Astronomy, Brigham Young University, Provo, UT 84602, USA

We propose an approach to materials prediction that uses a machine-learning interatomic potential to approximate quantum-mechanical energies and an active learning algorithm for the automatic selection of an optimal training dataset.

Our approach significantly reduces the amount of density functional theory (DFT) calculations needed, resorting to DFT only to produce the training data, while structural optimization is performed using the interatomic potentials.

Our approach is not limited to one (or a small number of) lattice types (as is the case for cluster expansion, for example) and can predict structures with lattice types not present in the training dataset. We demonstrate the effectiveness of our algorithm by predicting the convex hulls for the following three systems: Cu-Pd, Co-Nb-V, and Al-Ni-Ti. Our method is three to four orders of magnitude faster than conventional high-throughput DFT calculations and explores a wider range of materials. In all three systems, we found unreported stable structures compared to the AFLOW database.

MM 4.3 Mon 10:45 H45

Automated error analysis and control for ab initio calculations — •Jan Janssen, Tilmann Hickel, and Joerg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Over the last years methodological and computational progress in atomistic simulations have substantially improved the predictive power in materials design. A critical prerequisite to ensure a reliable comparison between the ab initio computed data with experimental data is to quantify the various sources of uncertainty present in the ab initio calculations. These include systematical errors due to insufficient convergence, statistical or numerical errors due to incomplete sampling and model errors for derived quantities. A well-known example is the determination of the equilibrium lattice constant and bulk modulus, which requires a careful analysis of the fit of the ab initio data on an approximate analytic form such as the Murnaghan equation of state.

To automatize the complex analysis we have developed an algorithm which takes the precision in the derived quantity as a convergence goal and automatically determines the convergence parameter to achieve it.

This algorithm is implemented using pyiron (http://pyiron.org) - an integrated development environment (IDE) for computational material science. This tool provides an efficient and user friendly environment to implement complex simulation protocols and allows to run them as high-throughput simulations over the periodic table. Our investigations revealed that many of the commonly used rules of the thumb for fitting ground state materials properties become invalid for high precision calculations.

MM 4.4 Mon 11:00 H45

Flexible and User-friendly Symmetry-Constrained Optimization and its Application to Study Different SiO$_2$ Polymorphs — •Sara Panahian Jand[1], Maja-Olivia Lenz[1], David Hicks[2], Stefano Curtarolo[2], Matthias Scheffler[1], and Christian Carbogno[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Duke University, Durham NC, USA

In computational solid-state physics, crystal symmetries are frequently exploited to accelerate and improve electronic-structure calculations. However, the standard techniques are usually not applicable when the global symmetry is broken, e.g, in defective materials or thermodynamic investigations. To overcome this problem, we have developed and implemented flexible geometry-constrained relaxation in the all-electron code FHI-aims. This approach preserves the *local* symmetries on a per-atom basis via user-defined symmetry-reduced parameters as presented in the AFLOW library of prototypes [1]. We demonstrate the flexibility and power of the approach by studying the stabilities of different SiO$_2$ polymorphs. For this compound, it is generally difficult to model structural transitions at very high temperatures and/or pressures [2]. However, our method provides a rapid way to compute the phase diagram of SiO$_2$, including the temperature-dependent lattice expansion. This demonstrates the ability of the developed approach to aid and accelerate the systematic search for metastable structures and the calculation of their thermodynamic properties.
[1] M. J. Mehl, *et al.*, *Comp. Mater. Sci.* **136**, S1 (2017).
[2] C. Catlow, *et al.*, *Phys. Chem. Chem. Phys.*, **12**, 786 (2010).

MM 4.5 Mon 11:15 H45

Uncertainty Quantification Framework for Force-Matched Classical Potentials — •Peter Brommer and Sarah Longbottom — University of Warwick, Coventry, UK

Classical effective potentials, where the energy of the system (and thus the forces on the atoms) only depend on the atomic positions, underpin a significant fraction of molecular dynamics (MD) simulations. Unfortunately, the bias, approximations and uncertainties incurred when representing the complex energy landscape by an effective potential or force field with a limited number of parameters are badly controlled, and the impact on quantities of interest (QoI) of an MD simulation is *a priori* unknown.

For potentials obtained by force matching, i.e. by adjusting their parameters to optimally reproduce forces, stresses and energies from first-principles calculations, we present an extension to the force-matching package *potfit*, where the uncertainty in the parameter set is encapsulated in an ensemble of potentials. This allows propagation of the uncertainty to QoI and makes uncertainty quantification accessible to users. We demonstrate this capability using three distinct potentials for Nickel and determine predictions and confidence intervals for lattice constants, elastic constants and thermal expansion.

15 min. break

MM 4.6 Mon 11:45 H45

On finding the dipole in the haystack of MD trajectories — •Frederic Felsen, David Egger, and Christoph Scheurer — Theoretical Chemistry, Technical University Munich

Aiming at implicit solvation models for large scale simulations of chemical reactions, we took a first step in the development of an automated solvent characterization based on classical MD trajectories. By modifying a method for the detection of semi-rigid domains in macromolecular structures [1], we propose a coarse graining procedure for decomposing a charge neutral atomistic system into a multi-center dipole

representation. The procedure is formulated in terms of a series of linearly constrained quadratic programming problems, which describe a clustering of the particles with respect to three major properties: spatial compactness, as the multi-center expansion is in terms of ideal point dipoles, structural rigidity, to ensure a valid mapping over the whole trajectory, and local charge neutrality. Solving these optimization problems by means of an active set algorithm yields the dipole domain decomposition of the system of interest. Based on such a dipole representation, an expression for the system's polarization can be obtained which is directly related to the dielectric function of the medium [2]. Investigating molecular (liquids and macromolecules) as well as crystalline (MoS_2 sheet structures) test systems, the key features of the coarse graining will be discussed.

[1] S. Bernhard, F. Noé, PLOS ONE, 5, (2010).
[2] D. Bonthuis, S. Gekle, R. Netz, *Langmuir*, 28(20), (2012).

MM 4.7   Mon 12:00   H45
Looking for Needles in the Haystack with Fuzzy Glasses: Screening Crystal Structures with Approximate Electronic Structure Methods — •Simon Wengert, Chiara Panosetti, Johannes T. Margraf, and Karsten Reuter — Technische Universität München, Germany

Still largely a Holy Grail of modelling, the capability to reliably predict the structure of (molecular) crystals would allow for the *in silico* design of substances with desired characteristics. Application fields range from dissolution properties (and consequently the bioavailability) of drugs to optoelectronic properties in organic photovoltaics. The main challenges in this respect are the large number of possible polymorphs and the small energy differences between them. In practice, there is thus a trade-off between the ability to screen a wide range of candidates (which requires some fast evaluation of stability) and applying levels of theory that adequately describe the interplay between subtle intermolecular interactions such as H-bonding, electrostatic and dispersion effects.

Dispersion-corrected density-functional theory (DFT) is typically considered to be sufficiently accurate for this purpose, but too expensive for routine global structural screening applications. We therefore compare two approximate DFT-models, namely the Harris approximation and density-functional tight-binding (DFTB) with respect to their efficiency and accuracy. We find that DFTB is surprisingly accurate, yielding mostly correct rankings in the targeted low-energy range. The errors of both approaches are discussed in depth.

MM 4.8   Mon 12:15   H45
Screening of rare-earth-lean intermetallic 1-11-X, 1-12-X, and 1-13-X compounds for hard-magnetic applications — Wolfgang Körner[1], •Daniel F. Urban[1], and Christian Elsässer[1,2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]University of Freiburg, FMF, Germany

We report on comparative theoretical investigations of ferromagnetic rare-earth-transition-metal phases with underlying YNi_9In_2 ("1-11"), $ThMn_{12}$ ("1-12") , and $LaCo_9Si_4$ ("1-13") crystal structures. By a combinatorial high-throughput-screening (HTS) approach based on density functional theory the intrinsic key properties of hard magnets, namely the magnetization M, energy product $(BH)_{max}$ and uniaxial magnetocrystalline anisotropy constant K_1 are estimated [1,2]. We interpret the results in terms of the differences in the three structure types and analyze the effect of additional light interstitial atoms (X = B, C, N). In the HTS study, which considers Ce, Nd or Sm as rare-earth elements and Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Al, Si, and P on the transition metal sites, several promising phases are identified which partially outperform $Nd_2Fe_{14}B$ in terms of $(BH)_{max}$ and K_1 values, and contain significantly less rare-earth atoms.

[1] W. Körner, G. Krugel, and C. Elsässer, Sci. Rep. 6, 24686 (2016).
[2] W. Körner, G. Krugel, D. F. Urban and C. Elsässer, Scripta Mat. 154, 295 (2018).

MM 4.9   Mon 12:30   H45

A local Bayesian optimizer for atomic structures — •Estefanía Garijo del Río, Jens Jørgen Mortensen, and Karsten Wedel Jacobsen — CAMD, Department of Physics, Technical University of Denmark

A local optimization method based on Bayesian Gaussian Processes is developed and applied to atomic structures. The method is applied to a variety of systems including molecules, clusters, bulk materials, and molecules at surfaces. The approach is seen to compare favorably to standard optimization algorithms like conjugate gradient or BFGS in most cases. The method relies on prediction of surrogate potential energy surfaces, which are fast to optimize, and which are gradually improved as the calculation proceeds. The method includes a few hyperparameters, the optimization of which may lead to further improvements of the computational speed.

MM 4.10   Mon 12:45   H45
Machine learning enhanced atomistic simulation of ZrB2 at ultra-high temperatures — •Yanhui Zhang, Alessandro Lunghi, and Stefano Sanvito — School of Physics and CRANN, Trinity College Dublin, Dublin, Ireland

Machine-learned interatomic potentials (MLIP) are emerging as the tool of choice for molecular dynamics, since they exhibit robustness in large-scale atomistic simulations at a quasi-ab initio accuracy. Here we demonstrate the construction of such MLIP for the long-standing problem of extracting high-temperature properties of ultra-high temperature ceramics (UHTCs). Although some effort has been devoted in the past decades, the atomistic simulation at high temperatures is still sluggish. The development of a MLIP for UHTCs rises major challenges since it must simultaneously describe: 1) the constituent elements being much different from each other; 2) the nature of the bonding arising from a mixture of metallic, covalent and ionic interaction, 3) the complex response to heat and deformation loads, 4) the transferability across a wide range of temperatures and strains. All these attributes are extremely important for the accurate prediction of fundamental physical properties of UHTCs. We have developed a powerful MLIP using the SNAP model, which bears excellent temperature transferability. Thereafter, we have applied it to study the performances of UHTCs under heat and strain loads. Our simulations extend to temperature (up to 3000 K) far beyond what available in measurements. This work demonstrates that MLIPs are a very promising simulation tool in the field of ultra-high temperature materials.

MM 4.11   Mon 13:00   H45
SnP anodes for potassium-ion batteries: insights from computational structure prediction — •Matthew Evans[1], Kent Griffith[2,3], and Andrew Morris[4] — [1]TCM Group, Cavendish Laboratory, University of Cambridge, UK — [2]Department of Chemistry, University of Cambridge, UK — [3]Department of Materials Science and Engineering, Northwestern University, USA — [4]School of Metallurgy and Materials, University of Birmingham, UK

Replacing Li with more abundant alkali metals, Na and K, should decrease and stabilise the production cost of rechargeable batteries. One hurdle to overcome for Na- and K-ion batteries is the poor performance and capacity of carbonaceous anodes relative to those used in Li batteries. Alloying or conversion anodes provide an alternative route, provided destructive volume changes and resulting nanoparticle pulverisation can be mitigated.

In this talk, we shall present a computational crystal structure prediction study on the K-Sn-P ternary system, following recent experimental interest in Sn/P as conversion anodes for K-ion batteries. Using a combination of *ab initio* random structure searching (AIRSS), data mining and evolutionary approaches, several new stable crystal structures have been discovered. These structures are used to aid interpretation of ambiguous experimental results using the matador package (https://matador-db.readthedocs.io). Theoretical capacities of the two stable anode materials, SnP_3 and Sn_4P_3, are predicted to increase relative to the known phases by 31% and 19% respectively, with the novel ternary phases providing a route to minimise volume expansion.

MM 5: Mechanical Properties

Mechanical Properties I and II

Time: Monday 10:15–13:00   Location: H46

MM 5.1   Mon 10:15   H46

Grain structure and mechanical properties of the Cu-Al hybrid materials processed by High Pressure Torsion Extrusion — Dayan Nugmanov, Roman Kulagin, Horst Hahn, and ●Yulia Ivanisenko — Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), 76021 Karlsruhe, Germany

A comparative analysis of the microstructure and mechanical properties of Cu-Al hybrid samples with three different geometry configurations processed by High Pressure Torsion Extrusion (HPTE) had been performed. The HPTE technique allows to achieve large strains (up to 30) during just one pass in large-scale rod specimens with the diameter of 10 mm and the length of 35 mm. Room temperature tensile tests had shown an interesting two-stage mechanical behavior correspondent to the Cu-matrix and Al-wires tension processes. It was found that Al wires embedded in the ultrafinegrained (grain size less than one micrometer) Cu matrix got thinned as a result of HPTE, upon that wire thickness depends on its distance from the sample center. In specimen areas corresponding to the middle-radius initially one mm in diameter wires were thinned to the tapes with the thickness of 20-30 micrometers, whereas in the edge areas their thickness was two-three micrometers, which reflects the strain gradient at HPTE.

MM 5.2   Mon 10:30   H46

Plastic deformation of tungsten due to deuterium plasma exposure: Insights from micropillar compression tests — ●Xufei Fang[1], Marcin Rasinski[2], Arkadi Kreter[2], Christoph Kirchlechner[1], Christian Linsmeier[2], Gerhard Dehm[1], and Steffen Brinckmann[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — [2]Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

The understanding of hydrogen embrittlement in metals is of importance for the failure prediction in components. Previous nanoindentation tests have shown that exposure to deuterium (D) plasma causes a decrease in pop-in load and an increase in hardness of tungsten. In this work, we use micropillar compression to investigate the plastic deformation and apparent strain hardening of tungsten exposed to D. In comparison to reference pillars, the pillars tested after exposure showed an increased apparent strain hardening rate as well as an increased multitude of slip traces. These outcomes are attributed to the presence of D that impedes the dislocation motion. Different loading rates in micropillar compression shed light on the competing mechanisms of dislocation and D mobility.

MM 5.3   Mon 10:45   H46

Mechanical properties of CrN-based nitride superlattices from ab inito calculations — ●Lukas Löfler[1], Paul Heinz Mayerhofer[2], Matthias Bartosik[2], and David Holec[1] — [1]Montanuniversität Leoben, Leoben, Austria — [2]TU Wien, Vienna, Austria

Thin film coatings are used to protect surfaces of tools and components from harsh environmental and/or though pplication conditions. Next to changing the composition, a new way to tune material properties is to carefully create a microstructural design for the material. The simplest way are (semi-) coherent multilayers with a bi-layer period in the nm range. At certain thicknesses the materials show a significant increase in hardness and fracture toughness, two material properties relevant for many applications.

At such small scales the interface has an increasing influence on the overallproperties of the material. Density Functional Theory (DFT) is a potent technique to describe these superlattices and investigate their mechanical properties. CrN, a common coating material, was paired with AlN and TiN to form superlattices. At first, the elastic constants of different interface orientations were determined. Further, the critical tensile strength at and near those interfaces were calculated. To correlate the results to experiments, the KIC values in and perpendicular to the interface directions were calculated.

MM 5.4   Mon 11:00   H46

Effect of grain boundary morphology on crack propagation behaviour in Tungsten — ●Shivraj Karewar and Erik Bitzek

— Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), Materials Science & Engineering, Institute I

Grain boundaries (GBs) in metals are commonly seen as preferential sites for crack nucleation and propagation. It has been shown that the atomic arrangements at GBs can affect the crack propagation [J. J. Möller, E. Bitzek, Acta Mat., 73, 2014, 1]. The atomic arrangement, in turn, depends on the misorientation, the GB plane, but also on GB defects like ledges and consequently on GB curvature.

Here we present the results of atomistic fracture simulations along tilt GBs in Tungsten. Crack propagation was studied for planar GBs of identical misorientation but different plane normals, as well as for curved GBs containing locally the same GB planes. Crack propagation for different GB misorientations were also investigated. In addition to quasi 2D simulations with minimal crack front length, simulations of extended crack fronts interacting with localized GB protrusions were performed. The results are discussed in terms of the plane-dependent GB energy, fracture surface area and the local stress state at GB defects.

MM 5.5   Mon 11:15   H46

Molecular dynamics investigation of size effects in lamellar γ-based TiAl alloys — ●Ashish Chauniyal, Alexander Hartmaier, and Rebecca Janisch — ICAMS,Ruhr-Universität Bochum

Two-phase γ-based TiAl alloys with a lamellar microstructure are interesting candidates for high temperature structural applications, due to a beneficial combination of creep resistance and fracture toughness. These microstructures consist of the α_2-Ti$_3$Al and γ-TiAl phases, which can be as finely spaced as several tens of nanometers. The thickness and distribution of these phases in such nano-lamellar alloys is a dominant factor dictating their hardness, which increases with decreasing lamellae spacing. However, nanoindentation tests are limited by the indenter size which indents over several lamellae simultaneously and provides only an averaged value of local hardness. Furthermore, the dynamics in nano scale is hard to capture and is mostly speculative based on pre- and post-indentation images. Using large scale atomistic simulations, indents can be made on individual lamellae using small indenters, which allows us to decouple the individual influence of lamella thickness, spacing and lamella phase on the hardness of the samples. In this study we carry out molecular dynamics nanoindentation simulations to identify the origins of the experimentally observed size effects. Furthermore, we focus on the evolution of dislocation activity underneath the indenter and correlate it with local and average hardness.

15 min. break

MM 5.6   Mon 11:45   H46

Influence of Post Annealing on The Microstructure and Mechanical Properties of CuSn4/Fe Nanolaminates produced by ARB — ●Maher Ghanem, Benoit Merle, Heinz Werner Höppel, and Mathias Göken — Friedrich Alexander Universität (FAU)_Lehrstuhl WW1: Allgemeine Werkstoffeigenschaften

The accumulative roll bonding (ARB) process has been applied to produce laminates with a layer thickness in the submicron to nanometer range. CuSn4/Fe nanolaminates with alternating layers of CuSn4 and Fe (99.88%) were produced by roll-bonding with 50% reduction and annealing at 400 *C following each pass. The rolling was repeated 14 times to achieve a layer thickness of about 100 nm. These nanolaminates were post annealed at different temperatures and the changes in their microstructure and mechanical properties as the number of ARB passes increased were observed. The microstructure was evaluated by means of backscatter electron (BSE) imaging and the mechanical properties of the nanolaminates were investigated through tensile and nanoindentation tests in order to observe the changes both locally and globally. It was found that the strength of the laminated composite could increase by a factor of about 2.5 times compared to single components. This increase in strength is discussed in terms of microstructural and phase interface contributions.

MM 5.7   Mon 12:00   H46

Adhesive wear mechanisms in the presence of weak interfaces — •Tobias Brink and Jean-François Molinari — Civil Engineering Institute and Institute of Materials Science and Engineering, EPFL, Lausanne, Switzerland

Despite the relevance of wear in many engineering applications, our understanding of the connection between mechanisms at the nanoscale and the observed wear rates of contacting parts at the macroscale remains limited. Recent work in our group has therefore focused on physics-based models of adhesive wear mechanisms, identifying a material-dependent critical length scale for wear particle formation [1]. Upscaling of these findings, though, still remains challenging [2]. One problem is that only strong adhesive bonds between contacting solids were considered. In the present contribution, we therefore extent this framework to include weaker interfaces, which are expected at typical contacts due to lattice mismatch, surface passivation, or lubrication. We use atomistic simulations on an amorphous model material to propose a mechanism map based on material properties and local contact geometry for wear particle formation and surface damage at the single-asperity scale. Our results imply that the local slopes of rough surfaces govern a transition from asperity collisions with plastic damage and wear particle formation at high roughness to slip without significant damage for flatter surfaces, comparable to a run-in process.

[1] Aghababaei, Warner, Molinari, Nat. Commun. **7**, 11816 (2016)
[2] Frérot, Aghababaei, Molinari, JMPS **114**, 172 (2018)

MM 5.8   Mon 12:15   H46
Electro-chemo-mechanical coupling of nanoporous gold at the microscale — •Yijuan Wu[1], Jürgen Markmann[1,2], and Erica Thea Lilleodden[1,3] — [1]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [2]Institute of Materials Research and Technology, Hamburg University of Technology, Hamburg, Germany — [3]Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany

The effect of variation of electrode potential on the micro-mechanical behavior of nanoporous gold (NPG) was investigated by in situ micro-compression in an electrochemical environment. Micro-pillars of NPG were produced by focused ion beam milling and then mechanically tested in an electrolyte using a nanoindenter equipped with a flat punch. Using a novel loading profile, the contribution to the measured displacement due to the actuation could be decoupled from the compression-induced deformation. The electro-chemo-mechanical coupling resulted in a considerable increase in the strength of the pillars when surface adsorption occurred, i.e. under positive applied potential, and the stress response to potential jumps was found to be fast and reversible.

MM 5.9   Mon 12:30   H46
Verifying Larché-Cahn theory by measuring open-system elasticity of nanoporous palladium(-gold)-hydrogen — •Shan Shi[1,2], Jürgen Markmann[1,2], and Jörg Weissmüller[2,1] — [1]Institut für Werkstoffforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht, Geesthacht — [2]Institut für Werkstoffphysik und -technologie, Technische Universität Hamburg, Hamburg

Monolithic samples of nanoporous metals are suitable for studying the mechanical behavior of nanostructured metals via conventional, macroscale mechanical testing approaches. Here, we synthesized monolithic nanoporous palladium (np Pd) and palladium-gold (np Pd-Au) samples with ligament sizes below 10 nm, which allow fast hydrogen redistribution across their diameter when stress gradients are induced by bending. The corresponding variation of the Young's modulus during hydrogen absorption/desorption is measured by a dynamic mechanical analyzer. It is found that hydrogen sorption enables more than 30% reversible compliance variation in np Pd. Moreover, the redistribution of hydrogen, i.e. the change of local hydrogen concentration inside the ligaments, during the deformation causes an additional reduction of the effective elastic coefficients in the single-phase regime of Pd(-Au)-H at low hydrogen concentration. The measured Young's modulus shows excellent agreement with the prediction by the Larché-Cahn theory of open-system elasticity.

MM 5.10   Mon 12:45   H46
Ferroelectric fracture ratchet effect caused by flexoelectricity — •Kumara Cordero-Edwards[1,2], Hoda Kianirad[3], Carlota Canalias[3], Jordi Sort[4,5], and Gustau Catalan[1,5] — [1]Catalan Institute of Nanoscience and Nanotechnology (ICN2), Barcelona, Catalonia — [2]DQMP, University of Geneva, Geneva, Switzerland — [3]KTH-Royal Institute of Technology, Stockholm, Sweden — [4]Universitat Autònoma de Barcelona (UAB), Bellaterra, Spain — [5]Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona, Catalonia

The propagation front of a crack generates large strain gradients and it is therefore a strong source of gradient-induced polarization (flexoelectricity). Fracture fronts generate flexoelectric fields that have an energy cost which, in turn, affects the mechanical response of materials. In ferroelectrics, this cost depends on the ferroelectric polarity. Therefore one can change the fracture toughness of a ferroelectric by switching its polarization.

Our work demonstrates experimentally that, as a consequence of flexoelectricity, crack propagation is promoted or diminished when directed parallel or antiparallel to the ferroelectric polarization, respectively. In addition, we have studied flexoelectrically induced domain switching around the crack, and showed that crack-induced flexoelectric switching is a contributor to the toughening of ferroelectrics with polarization antiparallel to the crack. The discovery of crack propagation asymmetry implies that fracture physics cannot be assumed to be symmetric in polar materials, and it demonstrates that flexoelectricity must be incorporated in any realistic model.

MM 6: Topical session (Symposium MM): Correlative and in-situ Microscopy in Materials Research

Advanced Characterization I

Time: Monday 11:45–13:15   Location: H44

Topical Talk   MM 6.1   Mon 11:45   H44
Break through new materials characterization frontiers with Atom Probe Microscopy — •François Vurpillot, Benjamin Klaes, Rodrigue Larde, Stefan Parviainen, and Bertrand Radiguet — Normandie Université, UNIROUEN, INSA Rouen, CNRS, Groupe de Physique des Matériaux, 76000 Rouen, France

Atom Probe Microscopy (APM) was proposed in 2012 [1] as a term that embraces the various techniques that derive from field emission generated by tip-like specimen. The most popular and fashion technique of APM is certainly the Atom Probe Tomography (APT) as evidenced by the dramatic increase in the number of books and publications in this field [1-4]. If now APT has its place among the panel of microscopy techniques, this instrument reaches its frontiers due in part to instrumental limitations, but more fundamentally intrinsic physical limitations. Break through these frontiers is however possible by correlating experimental data with accurate modelling and simulation approaches. This presentation will focus on different examples showing the capabilities of APM to image atomic defects in 3D and in the real space. The impact of the stress induced by the high field application is discussed from the quantum scale to the mesoscopic scale.

[1]*B. Gault et al., Atom Probe Microscopy, Springer, 2012. [2]*Lefebvre et al., Atom Probe Tomography Put Theory Into Practice, Academic Press, 2016. ; Larson et al.., Local Electrode Atom Probe Tomography, A User's Guide, Springer, 2013 ; Miller and Forbes, Atom-Probe Tomography, The Local Electrode Atom Probe, Springer, 2014

MM 6.2   Mon 12:15   H44
Determination of 3D electrostatic field at an electron nano-emitter — •Mingjian Wu[1], Alexander Tafel[2], Peter Hommelhoff[2], and Erdmann Spiecker[1] — [1]Institute of Micro- and Nanostructure Research & Center for Nanoanalysis and Electron Microscopy (CENEM), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen — [2]Department Physik,

Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen

Revealing and quantifying the 3D electrostatic field of field emission nano-emitters is key to answer the fundamental question of how the field interacts with the sharp tips. Here, we determine the 3D electrostatic field in situ at an electron nano-emitter. Differential phase contrast in scanning transmission electron microscopy has been applied to image nanoscale electrostatic fields of a sharp tungsten electron emitter with an apex radius of about 20 nm and under field emission condition. Assuming axial symmetry of the nano-emitter, we derived a method based on the inverse Abel transform to quantitatively reconstruct an axial slice of the 3D electrostatic field from a single projection measurement. The highest field strength of 2.92 V/nm is measured at the nano-emitter apex under condition of a bias voltage of -140 V with respect to the grounded counter electrode located about 650 nm from the apex, resulting in an emission current of more than 2 uA. The experimental results are compared with simulations based on a finite element numerical Maxwell equation solver. Quantitative agreement between experiment and simulation has been achieved.

MM 6.3 Mon 12:30 H44
Cryo-atom probe tomography for in-situ diffusion measurement of H at crystal defects — •Peter Felfer — Institute for General Materials Properties, Department of Materials Science, Friedrich-Alexander Universität Erlangen-Nürnberg

The diffusion of H in metallic materials is a highly important phenomenon in for both hydrogen energy conversion and structural integrity of materials. Historically, diffusion experiments at the crystal defect scale have not been possible due to measurement instrumentation limitations. As a result, the theoretical description of the phenomenon lacks experimental data to be compared to on individual defects. In recent years atom probe tomography has shown to be capable of delivering such data. About a decade ago atom probe has first been used to locate H, more specifically D in metals. Initially, deuteration through gas charging was used to create D dissolution in thermodynamic equilibrium, which was then supplemented by electrochemical charging, which can be used to create supersaturated states. Since for Fe, the most common base metal in engineering in the form of steel, has very low residual solubility for H even at room temperature, but still a high diffusion coefficient, cryo-cooling can be used to *freeze* D in the material and trigger diffusion only at controlled time intervals. In this talk, I will present first results of such a diffusion experiment. I will also present the design and first results of direct H (no D) measurements in metallic materials using a new atom probe with very low H background.

MM 6.4 Mon 12:45 H44
Atom Probe Tomography for Thermoelectric Materials — •Yuan Yu[1], Oana Cojocaru-Mirédin[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen Univeristy, Som-

merfeldstraße, 52074 Aachen, Germany — [2]JARA-Institut Green IT, JARA-FIT, Forschungszentrum Jülich GmbH and RWTH Aachen University, 52056 Aachen, Germany

Both microstructures and chemical composition of defects, including 0D point defects, 1D dislocations, 2D interfaces, and 3D precipitates, significantly influence the electrical and thermal transport properties of thermoelectric materials. However, determining their three-dimensional chemical composition, with a spatial accuracy of sub-nanometer and chemical sensitivity of ~10 ppm was impossible until the emergence of atom probe tomography (APT). In this work, we summarize the existing studies on local composition of various structural defects in thermoelectric materials using APT. With the chemical information at sub-nanometer scale, the corresponding thermoelectric properties can be better understood. Moreover, APT can distinguish a peculiar bonding mechanism, which is called metavalent bonding being responsible for intrinsic low lattice thermal conductivity, between matrix and defects. This provides a novel method to analyze and adjust the tradeoff between intrinsic bonding and extrinsic defects. Thereby, this precious technique is able to extend the concept of defect engineering and adjust the balance between bonding and defects in thermoelectrics and facilitate the rational design of high-performance thermoelectric materials.

MM 6.5 Mon 13:00 H44
Magic Colloidal Clusters: 3D Investigation of Self-assembled Polystyrene Particles forming Agglomerations in Crystalline Order using X-Ray Nano- and Electron Tomography — •Silvan Englisch[1], Janis Wirth[1], Thomas Pryzbilla[1], Benjamin Apeleo Zubiri[1], Junwei Wang[2], Nicolas Vogel[2], and Erdmann Spiecker[1] — [1]Institute of Micro- and Nanostructure Research , Friedrich Alexander-University of Erlangen-Nuremberg (FAU), Germany — [2]Institute of Particle Technology at the FAU

X-ray tomography (XRT) and electron tomography (ET) allow 3D investigations across multiple length scales. Morphological segmentation of the tomographic reconstructions of complex sample structures enables in-depth quantitative and position-correlating analyses. So-called magic colloidal clusters are self-organized structures (or assembies) of polystyrene colloidal particles. XRT/ET were employed to study the exact 3D positions of each individual primary particle. A sufficiently high contrast in the acquired reconstructions, which is important for a reliable segmentation of the 3D datasets, is challenging to achieve since the samples are reaching the limits of XRT (resolution) and ET (size). On the one side, a morphology-threshold filter (software: Arivis) was applied to segment the original reconstructions and determine the 3D positions of the spherical and monodisperse primary particles. On the other side, spheres with a particle-size matching diameter were fitted to these positions in a virtual volume. These workflows allow to investigate the exact structure and possible defects in such magic colloidal clusters.

MM 7: Invited talk Erhart

Time: Monday 15:00–15:30   Location: H43

Invited Talk   MM 7.1 Mon 15:00 H43
Thermodynamics and optical response of nanoscale systems from atomistic simulations — •Paul Erhart[1], Tuomas Rossi[1], Magnus Rahm[1], and Mikael Kuisma[2] — [1]Chalmers University of Technology, Department of Physics — [2]University of Jyväskylä, Department of Chemistry

The properties of nanoparticles are sensitive to size, shape, composition, and environment, providing ample opportunities for material optimization and targeted design of functionalities. Here, I will summarize recent work from my group that addresses thermodynamic and optical properties of metallic nanoparticles.

Atomic scale simulations reveal an energy landscape as a function of size and shape that is more intricate than previously suggested. The

thus obtained particle type distributions demonstrate that the transition from icosahedral particles to decahedral and further into truncated octahedral particles occurs only very gradually, which has implications for the interpretation of experimental data.

Metal nanoparticles can also support localized surface plasmon resonances, which can decay into high-energy electrons and holes allowing hot-carrier generation for, e.g., photocatalysis. In this context, I will show ongoing work in which we follow plasmon formation as a collective excitation, track its subsequent decay into incoherent electron-hole transitions, and finally, obtain the corresponding hot-carrier distributions. Our work paves the way for addressing the spatiotemporal dynamics of hot-carrier generation in catalytically-relevant edge and corner sites of nanoparticles.

MM 8: Topical session (Symposium MM): High entropy and compositionally complex alloys

Sessions: Modelling I and II

Time: Monday 15:45–18:30   Location: H43

Topical Talk   MM 8.1   Mon 15:45   H43
First principles modeling of high entropy alloys — •Levente
Vitos — Royal Institute of Technology KTH, Stockholm, Sweden

Thanks to impressive developments within Density Functional Theory
(DFT), electronic structure solvers and computational power during
the last few decades, modern materials research receives increasing sup-
port from first-principles modeling. Such approach gives fundamental
understanding, offers efficient pre-screening against various degrees of
freedom and provides information where experimental assessments are
not feasible. Today the ab initio theory aided materials assay finds its
way in almost all areas of advanced materials design and characteriza-
tion.

Due to the complexity of the problem, DFT modeling was practi-
cally missing within the field of High Entropy Alloys (HEAs) for almost
one decade after their discovery. Starting from early 2010s, we made
a series of attempts to fill this gap and extend the scope of ab initio
modeling to HEAs. In the present contribution, I will briefly overview
the pioneering applications of alloy theory in the case of magnetic and
refractory HEAs, and point out the main known and hidden challenges
associated with such efforts. I will present our recent theoretical pre-
dictions for the mechanical and magnetic properties of existing and
hypothetical HEAs. Special emphasis will be places on the plastic
deformation mechanism in HEAs with close packed crystal structure
and the role of intrinsic energy barriers in the competing deformation
mechanisms.

MM 8.2   Mon 16:15   H43
**The elastic-strain energy stability criterion for complex con-
centrated alloys** — •Angelo F Andreoli[1], Jiri Orava[1], Peter
K Liaw[2], Hans Weber[1], Marcelo F de Oliveira[3], Kornelius
Nielsch[4], and Ivan Kaban[1] — [1]IFW Dresden, Institute for Complex
Materials, Helmholtzstr. 20, 01069 Dresden, Germany — [2]Materials
Science and Engineering Department, The University of Tennessee, 414
Ferris Hall, Knoxville, TN 37996, USA — [3]Materials Science and En-
gineering Department, University of São Paulo, Avenida João Dagnone
1100, CEP 13563-120, São Carlos, SP, Brazil — [4]IFW Dresden, Insti-
tute for Metallic Materials, Helmholtzstr. 20, 01069 Dresden, Germany

An empirical method is developed, based on the calculated theoretical
elastic-strain energy, to predict the phase formation and its stabil-
ity for complex concentrated alloys. The method prediction quality
is compared with the traditional empirical rules based on atomic-size
mismatch, enthalpy of mixing and valence electron concentration for
a database of 235 different alloys. Considering the different available
empirical methods used to date, the *elastic-strain energy vs. valence
electron concentration* criterion shows an improved ability to distin-
guish between single-phase solid solutions, mixtures of solid solutions
and intermetallic phases. The criterion is especially strong for alloys
that precipitate the mu phase. The theoretical elastic-strain-energy
parameter can be combined with other known parameters, such as
those noted above, to establish new criteria which can help predicting
the design of novel high-entropy alloys with on-demand combination
of mechanical properties.

MM 8.3   Mon 16:30   H43
Ab initio **vibrational free energies including anharmonic-
ity for multicomponent alloys** — •Prashanth Srinivasan[1],
Yuji Ikeda[2], Blazej Grabowski[2], Jan Janssen[2], Alexander
Shapeev[3], Jörg Neugebauer[2], and Fritz Körmann[1,2] — [1]TU
Delft — [2]MPIE Dusseldorf — [3]Skolkovo Institute of Science and Tech-
nology

High entropy alloys have gained widespread attention owing to their
superior mechanical properties. *Ab inito* modeling is a powerful tool to
analyze and predict their thermodynamic properties. In combination
with statistical sampling techniques, free energy surfaces $F(T,V)$ are
accessible from which properties such as thermal expansion coefficient
and heat capacity can be derived and compared to experiments. At
higher temperatures, the vibrational free energy — including anhar-
monic contributions — is a major contributor. But as the number
of components in the alloy increases, *ab initio* calculations to obtain
accurate values of the free energy become expensive. In this work, we

present an efficient approach to numerically calculate exact vibrational
free energies. Firstly, a machine learnt potential (moment tensor po-
tential [Shapeev, 2016]) is built based on *ab initio* data, the validity
of which is tested by comparing its results to DFT, and secondly, the
MTP is used as a part of a thermodynamic integration to get accu-
rate vibrational free energies. The approach is applied to 12 refractory
alloys having two to five components to study the impact of config-
urational entropy on the vibrational free energies. The workflow is
implemented in pyiron (http://pyiron.org) to enhance its dissemina-
tion and reuse.

MM 8.4   Mon 16:45   H43
**Atomistic Simulation of Dislocations in High Entropy Al-
loys** — •Aviral Vaid[1], Michael Zaiser[2], and Erik Bitzek[1] —
[1]Materials Science and Engineering, Institute I, Friedrich-Alexander
Universität Erlangen-Nürnberg, Germany — [2]Institute of Materi-
als Simulation, Department of Materials Science, Friedrich-Alexander
Universität Erlangen-Nürnberg, Germany

Understanding dislocation mobility and dislocation-obstacle interac-
tions is of fundamental importance for the development of alloys with
improved mechanical properties. Single phase high entropy alloys
(HEAs) are a class of chemically complex alloys that have shown ex-
ceptional mechanical properties. Due to the chemical complexity of
these alloys, the characteristics of energy landscape that a dislocation
experiences in these alloys still needs to be investigated. Through
atomistic simulations, we perform a comprehensive characterization
of the segment-length-dependent dislocation properties such as Peierls
barrier, Larkin length, dislocation line energy, and dislocation struc-
ture for both edge and screw dislocations. The dislocations are studied
in model HEA systems using different potential formalisms to assess
the robustness of the atomistic simulation results. The random nature
of the pinning field, where in a sense every atom is a solute, leads to
a complex situation as the dislocation adjusts its shape to the fluc-
tuating energy landscape. The results are discussed in the context of
parametrizing discrete dislocation dynamics models.

30 min. break

Topical Talk   MM 8.5   Mon 17:30   H43
**Machine-learning interatomic potentials for multicomponent
alloys** — •Alexander Shapeev — Skolkovo Institute of Science and
Technology, Skolkovo Innovation Center, Moscow 143026, Russia

Multicomponent alloys are a challenge to materials design. It is time-
and resource-consuming to exhaust the space of possible compositions
experimentally, and equally time- and resource-consuming to do it via
ab initio modeling. Moreover, many empirical and data-driven ap-
proximants to ab initio models also fail because the configurational
space is huge and it is hard to avoid extrapolation when using such
approximants for modeling multicomponent alloys.

In my talk I will present a machine-learning framework for the dis-
covery of stable phases of multicomponent alloys and computation of
their free energy and derivative properties including thermodynamic
stability of phases. The framework is based on (1) machine-learning
interatomic potentials capable of very accurately approximating ab ini-
tio models, and (2) an active-learning algorithm capable of detecting
extrapolation in configurational space attempted when predicting in-
teratomic interaction, and through additional fitting ensure reliability
of the predictions.

MM 8.6   Mon 18:00   H43
**Tuning magnetic properties of high entropy alloys: A com-
bined theoretical and experimental study** — •Biswanath
Dutta[1], Ziyuan Rao[2], Lukas Schäfer[3], Zhiming Li[2], Oliver
Gutfleisch[3], Fritz Körmann[1,2], and Dierk Raabe[2] — [1]Materials
Science and Engineering, TU Delft, Delft, Netherlands — [2]Max-
Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany —
[3]Institut für Materialwissenschaft, TU Darmstadt, Germany

Magnetic properties of high entropy alloys (HEAs) have been a topic
of growing research in the last years. Of particular interest are subtle
changes in magnetic features due to the substitution of non-magnetic

elements in magnetic HEAs. Using ab initio calculations, we investigate the impact of Cu on magnetic properties of FCC FeCoNiMn alloys. The coherent potential approximation is employed to address the chemical disorder while the high temperature paramagnetic state is treated within the disordered local moment approach. Among the considered magnetic states, our calculations reveal an antiferromagnetic order for Mn atoms in the lowest energy state. The impact of this on the prediction of Curie temperatures is subsequently discussed. We show that both the Curie temperature and the saturation magnetization increase due to Cu substitution. The obtained compositional trends are discussed in terms of varying concentration of magnetic elements and volume changes. Our predicted trends of the magnetic properties also show excellent agreement with the corresponding experimental results. Based on the achieved results we identify Cu as a promising element to tune and improve magnetic properties of FeCoNiMn-based HEAs.

MM 8.7   Mon 18:15   H43
Investigation of phase stability in high-entropy alloys with the use of machine-learning interatomic potentials — •Tatiana Kostiuchenko[1], Alexander Shapeev[1], Fritz Körmann[2,3], and Jörg Neugebauer[2] — [1]Skolkovo Institute of Science and Technology,

Moscow, Russia — [2]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [3]Delft University of Technology,The Netherlands

High-entropy alloys (HEA) is a class of materials which consist of at least four different chemical elements and have a specific structure. These alloys have high ductility and yield strengthening, they are widely used as construction and heat-resistant materials. Experimental methods of HEAs investigation are time-consuming, and by this reason, computational methods of HEAs investigation are of the high interest. In this work, a new data-driven approach for investigation of solid solution stability in HEA is proposed. It is based on Canonical Monte Carlo algorithm with the use of machine-learning potential, namely low-rank potential (LRP) [Shapeev A., 2017]. The approach was examined by comparing it with the existing works. The key difference of the LRP from the other "on-lattice" models is its ability to take into account local lattice distortions, which is critical for the materials behavior. The parameters of the LRP were fitted on quantum-mechanical data, the LRPs prediction accuracy was 1 meV/atom. Thus, the temperature of the order/disorder phase transition was accurately calculated for the equiatomic NbMoTaW system. The low-energy structures and the mechanisms of chemical ordering were also investigated.

MM 9: Topical session (Symposium MM): Correlative and in-situ Microscopy in Materials Research

Sessions: Advanced Characterization II and III

Time: Monday 15:45–19:00   Location: H44

Topical Talk   MM 9.1   Mon 15:45   H44
Scanning transmission electron microscopy as a multidimensional information channel with spatial, momentum and time resolution — •Knut Müller-Caspary[1], Armand Beche[2], Florian Winkler[1], Florian Krause[3], Daen Jannis[2], Andreas Oelsner[4], Heike Soltau[5], Rafal Dunin-Borkowski[1], Sandra Van Aert[2], Johan Verbeeck[2], and Andreas Rosenauer[3] — [1]Forschungszentrum Jülich (D) — [2]EMAT Antwerpen (B) — [3]Universität Bremen (D) — [4]Surface Concept GmbH (D) — [5]PN Detector GmbH (D)

With the advent of ultrafast cameras, methodologies in the field of Scanning Transmission Electron Microscopy experienced a rapid development in the past 5 years. Pixelated STEM now enables the simultaneous acquisition of real and reciprocal space data at unprecedented resolutions and samplings. The methodological framework to measure electric fields at atomic and unit cell scale is presented, based on a robust measurement of the momentum transferred to the STEM probe by the interaction with specimen. We show experimental results on charge density maps in 2D materials and polarisation fields in piezoelectric specimen. Momentum-resolved STEM is additionally discussed as to its potential for the in-situ mapping of electronic properties in electrically biased devices, and the chemical composition mapping via an angular multi-range analysis. Moreover, we report current approaches to enhance the time resolution of ultrafast detectors to the ps-scale, and outline the new opportunities a high sampling of the time domain provides for the characterisation of materials and processes.

MM 9.2   Mon 16:15   H44
Scanning Transmission Electron Beam Induced Current Combined with Spectroscopy for Investigating Energy Conversion in Nanoscale Materials — •Tobias Meyer[1], Birte Kressdorf[2], Jonas Lindner[2], Patrick Peretzki[1], Vladimir Roddatis[2], Christian Jooss[2], and Michael Seibt[1] — [1]4th Institute of Physics: Solids and Nanostructures, University of Goettingen, Friedrich-Hund-Platz 1, 37077 Goettingen, Germany — [2]Institute of Materials Physics, University of Goettingen, Friedrich-Hund-Platz 1, 37077 Goettingen, Germany

Electron Beam Induced Current (EBIC) is a well-established, powerful characterisation tool in semiconductor physics which has been employed in Scanning Electron Microscopes (SEM) for decades, e.g. to map enhanced excess carrier recombination at crystal imperfections. Despite great advancements in instrumentation, the resolution of SEM based setups is rather limited since multiple scattering of the impinging electrons leads to a pear-shaped generation volume and hence a

sophisticated crosstalk between primary excitations and the sample's geometry.

Transferring the technique to the Scanning Transmission Electron Microscope (STEM), also referred to as Scanning Transmission EBIC (STEBIC), prevents the electron beam to spread significantly before exiting the sample. Thus, excess carrier dynamics on the nanometer scale become accessible and can additionally be correlated to state of the art STEM signals like Electron Energy Loss Spectra (EELS) and Nano Beam Electron Diffraction (NBED) patterns.

MM 9.3   Mon 16:30   H44
The influence of deformation on the medium-range order of a Zr-based bulk metallic glass characterized by variable resolution fluctuation electron microscopy — •Sven Hilke[1], Harald Rösner[1], David Geissler[2], Annett Gebert[2], Martin Peterlechner[1], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster, Germany — [2]Institute for Complex Materials (IKM), Leibniz-Institute for Solid State and Materials Research Dresden (IFW Dresden) Helmholtzstr. 20, D-01069 Dresden, Germany

The medium-range order (MRO) of both as-cast and deformed states of a Zr-based bulk metallic glass (Zr52.5Cu17.9Ni14.6Al10Ti5 (at.-%) - Vitreloy 105) were analyzed using variable resolution fluctuation electron microscopy (VR-FEM). Significant structural changes were observed in the MRO in regions close to and inside shear bands of deformed material, compared with that in the as-cast state (undeformed). As a result of deformation we conclude, that two distinct MRO cluster types were formed in both matrix and shear bands. Moreover, plastic deformation not only alters the MRO in terms of cluster size and volume fraction but also leads to a split into two distinct MRO types. The MRO length scale is larger inside the shear bands compared to the surrounding matrix, which indicates the impact of frictional heating and/or higher atomic mobility. Moreover, these results approve VR-FEM as a potential method for probing deformation stages even within the wide elastic regime of metallic glasses.

MM 9.4   Mon 16:45   H44
Simulation of fluctuation electron microscopy data: the Ka-Xi plot — •Martin Peterlechner, Sven Hilke, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Münster, Germany

The method of fluctuation electron microscopy (FEM), as introduced by Treacy and Gibson, is an excellent tool for analysis of amorphous materials. The signal of the ring intensity variation in a nano-beam

diffraction pattern (NBDP) along constant k-values ('Ka' values) is very sensitive to structural changes in the medium range order length scale. To understand the signal and gain knowledge on the sensitivity, we simulated NBDPs by a recently in-house developed multislice algorithm, STEMcl. For every beam position during a scanning transmission electron microscopy (STEM) experiment, the corresponding NBDP was segmented into 150 rings. The 150 corresponding STEM images were calculated, and the profiles of their Fouriertransforms were analysed ('Xi' space). The so obtained 'Ka-Xi' plots are analysed, and conclusions about optimum experimental conditions and the sensitivity of FEM in general are discussed.

MM 9.5   Mon 17:00   H44
Combined in situ heating and diffraction in Scanning Electron Microscopy — •Peter Denninger, Peter Schweizer, Christian Dolle, and Erdmann Spiecker — Friedrich-Alexander University Erlangen-Nuremberg, Cauerstrasse 6, 91058 Erlangen

In this work we introduce a novel heating and diffraction setup in the SEM enabling the simultaneous acquisition of real space and reciprocal space information in situ. Low Energy Nano Diffraction (LEND) in transmission is based on the combination of a fluorescent screen positioned below the sample with a dedicated CMOS camera. The technique has been implemented and successfully tested on graphene and polycrystalline gold. For graphene a hexagonal spot like diffraction pattern can be obtained due to the small convergence angle (hence nano diffraction) typically encountered in SEM. For gold the same is possible for very thin films. With increasing film thickness the contribution of dynamical scattering becomes more prevalent, resulting in familiar transmission Kikuchi diffraction (TKD) patterns. With our setup we could successfully demonstrate LEND down to an energy of 0.5 keV (hence low energy).

A custom-built heating stage for DENS Solution Wildfire Nano-Chips in combination with the LEND setup offers combined in situ heating, imaging and transmission diffraction in SEM. To showcase the power of this technique the process of solid state dewetting and the aluminum induced Layer Exchange (AlILE) will be shown. In both those processes the combined detection of real- and reciprocal space information lead to new insights about their mechanisms.

15 min. break

Topical Talk   MM 9.6   Mon 17:30   H44
Characterization of materials at the nanoscale using hard X-ray microspectroscopy techniques — •Gema Martinez-Criado — ICMM-CSIC, Calle Sor Juana Ines de la Cruz 3, 28049-Cantoblanco, Madrid, Spain

Hard X-ray spectromicroscopy techniques are key tools with relevant applications across multiple fields. In this presentation I briefly describe how these tools are implemented and correlated nowadays for the smart in-situ characterization of advanced heterogeneous materials at the nanoscale. In addition, the essential role of the associated instrumentation for reliable 2D and 3D data acquisitions with nanometer spatial resolution are shortly presented. Finally, few recent examples under operando conditions exemplify the potential of correlative hard X-ray modalities to provide new insights into nanostructures for novel nanodevices.

MM 9.7   Mon 18:00   H44
Revealing the Influence of Surfactants on the Fast Growth Kinetics of Organic Nanoparticles by In Situ Small-Angle Scattering Studies — •Dennis M. Noll, Isabel Schuldes, Torben Schindler, Tilo Schmutzler, and Tobias Unruh — Institute for Crystallography and Structural Physics, Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen, Germany

The combination of small-angle X-ray and neutron scattering (SAXS/SANS) with the stopped-flow technique allows for in situ studies of fast structure formation processes. The presented time-resolved experiments enable classical SANS in the regime of few milliseconds for the first time by performing and summing up hundreds of stroboscopic measurements for each sample system.

With in situ SAXS and SANS the fast growth of poorly-water soluble active pharmaceutical ingredient nanoparticles during the antisolvent precipitation process has been studied. To reveal the influence of surfactants on the growth kinetics and the ripening of the organic model system, precipitation with two structurally different and commonly used surfactants, as well as precipitation without any surfactant have

been studied. The results of the in situ SANS measurements show an early beginning of ripening already after 250 ms for all sample systems and increased growth kinetics for nanoparticles solubilized by micelles.

Additionally, first in situ SAXS and SANS results of a new and simple model system for small and long-term stable organic nanoparticles with a similar growth behavior will be presented.

MM 9.8   Mon 18:15   H44
In-operando studies on organic field-effect transistors — •Manuel Johnson[1], Tim Hawly[1], and Rainer H. Fink[1,2] — [1]Lehrstuhl für Physikalische Chemie II, FAU Erlangen-Nürnberg, Germany — [2]CENEM, FAU Erlangen-Nürnberg, Germany

Organic semiconducting films bear high potential for device applications such as field-effect transistors (OFETs). Understanding the correlation between microstructure and charge transport within the active layer of these devices is crucial to achieve high field-effect mobilities. To ad-dress this issue we performed spatially-resolved spectroscopic measurements to correlate the spectroscopic changes with the local microstructure of our thin organic film devices. In our studies we investigated pentacene and different thiophene derivative based OFETs. We could ob-serve small variations in the density of unoccupied states during device operation using X-ray microscopy and local NEXAFS spectroscopy. We attribute the spectral modifications in terms of intramolecular polarization for molecules located at the organic/insulator interface. Spatially-resolved XPS measurements offer additional insight into the absolute change in binding energy (BE). Our recent results contradict the findings from Nagamura et al. that conducted similar studies and reported a BE increase when applying a gate voltage [1]. We discuss the observed decrease in the BE with respect to the operation state of the OFET device and show that it can be used for a visualization of a charge accumulation layer inside the active layer. This research is funded by the DFG within GRK 1896.
[1] N. Nagamura, et al., Appl. Phys. Lett. 106, 2015, 251604

MM 9.9   Mon 18:30   H44
Structural studies on functional and solution-processed organic thin films — •Tim Hawly[1], Manuel Johnson[1], and Rainer Fink[1,2] — [1]Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]CENEM, Friederich-Alexander-Universität Erlangen-Nürnberg, Germany

State-of-the-art organic semiconducting layers offer a variety of advantages compared to conventional inorganic circuitry such as flexibility, low-cost processability and environmental compatibility. However, numerous experiments including vacuum-processed thin films in devices such as organic field-effect transistors (OFETs) suffer from diffusion-limited growth leading to polycrystalline films, which reduce high-mobility charge transport between the source and drain electrode. We utilized spatially resolved XPS to obtain insight into the operating, active layer of a typical OFET. We explored a novel preparation technique utilizing the surface of a liquid (most commonly water) as substrate.[1] Thin-film growth out of solution results in long-range ordered crystalline structures for a variety of small molecules and is ultimately capable of overcoming common domain sizes and grain boundaries present in vacuum-deposited films. Our findings are readily supported by microscopic (AFM, TEM), diffraction (SAED) and spectroscopic (Angle-resolved NEXAFS, STXM) techniques as well as by charge-transport measurements that excel reference data typically by one order in magnitude. This research is funded by the DFG within GRK1896. [1]: C. Xu et al., Angew. Chem. Int. Ed. 2016, 55, 9519-9523.

MM 9.10   Mon 18:45   H44
Structural analysis of complex Liquid Metal Catalyst structures utilizing 3D X-ray and Electron Microscopy — •Janis Wirth[1], Silvan Englisch[1], Christian Wiktor[1], Nicola Taccardi[2], Benjamin Apeleo Zubiri[1], Peter Wasserscheid[2], and Erdmann Spiecker[1] — [1]Institute of Micro- and Nanostructure Research (IMN) & Center for Nanoanalysis and Electron Microscopy (CENEM), Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Chair of Chemical Engineering I (Reaction Engineering), Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

X-ray microscopy (XRM) allows non-destructive 3D investigations of materials across multiple length scales. Due to the high-resolution capabilities and flexible contrast a correlative 3D study combined with scanning electron microscopy (SEM) and transmission electron microscopy (TEM) techniques is possible. In this contribution, we report about correlative 3D studies of Pd(Pt)-Ga liquid metal catalysts

which recently showed outstanding performance in alkane dehydrogenation and, in particular, high resistance against coking. This material exhibits a complex structure featuring a catalytically-active liquid film/droplet layer adsorbed on macroporous silica. 3D characterization across different length scales is required to gain deeper insight into the structure and microscopic mechanisms of the catalyst system. Utilizing XRM the metal droplets and the macroporous silica network can be independently resolved. In order to study the composition of individual metal droplets inside the porous network, site-specific sample preparation has to be combined with analytical TEM techniques.

MM 10: Methods in Computational Materials Modelling (methodological aspects, numerics)

Sessions: Atomic Potentials and Phonons

Time: Monday 15:45–18:45   Location: H45

MM 10.1 Mon 15:45 H45

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

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

In order to provide a generally applicable ACKS2 extension to force fields, we develop a new minimalistic basis set representation composed of s- and p-type Gaussian functions. We demonstrate the efficacy of ACKS2 with the new basis set for a range of molecular model systems including anthracene and tetracene, which are relevant building blocks in common organic semiconductors. Screening a range of external electrostatic perpurbations, we find very good agreement with density functional theory references. This marks an important first step to employ ACKS2 as polarization correction in force fields.

MM 10.2 Mon 16:00 H45

Validation and transferablity of interatomic potentials — •Yury Lysogorskiy, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr University Bochum, Germany

Interatomic potentials (IP) are widely used in computational materials science, in particular for simulations that are too computationally expensive for density functional theory (DFT). A large number of IPs is available for a wide range of chemical elements and their mixtures. Most IPs have a limited application range and often there is little information available regarding their performance for specific simulations.

We performed extensive tests for the majority of the potentials for unaries that are available from the OpenKIM and NIST repositories as well as from other sources. The following properties were considered: energy-volume curves, equilibrium bulk modulus, elastic constants, phonon spectrum and density of states, vacancy formation energies, transformation paths, surface energies, thermodynamic properties in the quasiharmonic approximation and thermal expansion. For accessing the transferability of IPs we cover a wide range of atomic environments by considering special random structures with one and two atoms in the unit cell and evaluated their energetic, geometrical and elastic properties. Two typical cases of IP behavior - high accuracy at the expense of low transferability versus low accuracy but higher transferability were identified. The results of our calculations are collected in a specially designed database for further analysis.

MM 10.3 Mon 16:15 H45

Parametrization of classical force fields for single molecule junctions — •Narendra P. Arasu and Hector Vazquez — Institute of Physics of the Czech Academy of Sciences, Cukrovarnicka 10, Prague, Czech Republic

In molecular junctions, where single molecule bridges the gap between metal electrodes, interface geometry under the influence of thermal fluctuations can be explored from Molecular Dynamics (MD) simulations. Ab-initio methods are accurate but their computational cost restricts the time scale that can be probed in the simulations. Thus, simulations based on Density Functional Theory (DFT) can be limited to rather restricted phase-space. On the other hand, Molecular Mechanics (MM) simulations are computationally faster than DFT. However, careful parametrization of the MM energy functions is required for realistic representation of an MD ensemble. In this work, we propose a method to parametrize Optimized Potentials for Liquid Simulations (OPLS-AA) forcefield to run a long time scale (˜ nanoseconds) MD simulations. The parameters are obtained by fitting the model energy functions of short-range interactions to the energies from DFT calculations. As a prototypical molecular junction, we consider a biphenyl molecule with three different linker groups having different chemical binding: Au-C, Au-NH2, and Au-SCH3 to test our parametrization technique. We compare the statistics of changes in bond lengths, angles and dihedrals obtained from classical MD trajectories to that of the ab-initio MD simulations. The results show that the parameters obtained using our method describe well DFT MD simulations.

MM 10.4 Mon 16:30 H45

Parametrization of a bond-order potential for Ti — •Alberto Ferrari, Malte Schröder, Yury Lysogorskiy, Jutta Rogal, Matous Mrovec, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, 44801 Bochum, Germany

Ti alloys are attractive structural materials, featuring remarkable stiffness/weight and strength/weight ratios, exceptional corrosion resistance, good creep properties, and biocompatibility. In addition, many Ti alloys exhibit shape-memory and superelastic properties, and the recently discovered gum-metals are also based primarily on Ti. Atomic-scale studies of Ti-based metals often employ first-principles methods such as density functional theory, with maximum system sizes that are limited to a few hundreds atoms. To perform large-scale and/or finite temperature simulations, empirical potentials or machine-learning potentials are usually fitted. However, the transferability of these potentials to properties or environments not included in the training is limited. In this contribution, we present a newly developed bond-order potential (BOP) for Ti derived by coarse-graining the tight-binding approximation to the electronic structure. The BOP model shows an unprecedented transferability to various bulk as well as defective Ti structures. We demonstrate the excellent predictive power of our potential for a number of structural and thermodynamic properties that are relevant for the structural stability, phase transformations, and defect behavior in Ti-based materials.

MM 10.5 Mon 16:45 H45

Learning to use the force: DFTB repulsion with Gaussian Process Regression — Artur Engelmann, •Chiara Panosetti, Johannes T. Margraf, and Karsten Reuter — Chair for Theoretical Chemistry, Technische Universität München, Germany

Density-Functional Tight Binding (DFTB) is increasingly popular among computational modellists as it provides comparable accuracy to DFT at a fraction of the cost, enabling large scale simulations while retaining direct access to electronic structure properties. Yet, a bottleneck to this day remains the difficulty to parametrize the interactions for large subsets of atoms across the periodic table, let alone an extensive, universal parametrization. Especially challenging is the parametrization of the pairwise repulsion: an unescapable N^2 effort, and a cumbersome one. Most schemes involve fitting the repulsion to some analytical potential by *e.g.* minimizing force residues. However, this presents a number of limitations, such as constraints on the reference geometries, and the necessity of projecting forces along the bonds. Further, any predefined functional form not only carries a certain degree of arbitrary bias in its very choice, but may also lack the flexibility to capture subtle features around equilibrium distances (where the "re-

pulsive" potential may as well be attractive). We thereby propose to rather machine-learn the repulsive force, using Gaussian Process Regression similarly to the generation of GAP potentials [1]. We discuss a proof-of-principle application on carbon, showing how such an approach removes all the above limitations at once.

[1] A.P. Bartók *et al.*, PRL 104, 136403 (2010)

MM 10.6   Mon 17:00   H45

A Neural Network Potential for Lithium Manganese Oxides — •MARCO ECKHOFF[1], PETER BLÖCHL[2], and JÖRG BEHLER[1] — [1]Universität Göttingen, Institut für Physikalische Chemie, Theoretische Chemie, Tammannstraße 6, 37077 Göttingen, Germany — [2]Technische Universität Clausthal, Institut für Theoretische Physik, Leibnizstraße 10, 38678 Clausthal-Zellerfeld, Germany

The lithium manganese oxide spinel $Li_xMn_2O_4$, with $0 < x < 2$, is an important cathode material in lithium ion batteries. Its accurate description by density functional theory (DFT) is far from trivial due to several energetically close electronic and magnetic states. In extensive benchmark studies we find that the hybrid functionals PBE0, HSE06, and PBE0r yield energetic, structural, electronic, and magnetic properties in good agreement with experiment. Building on such hybrid DFT, we are able to extend the time and length scales of molecular dynamics simulations of $Li_xMn_2O_4$ using a high-dimensional neural network potential, which provides a first-principles quality description of the potential energy surface at a fraction of the computational costs.

15 min. break

MM 10.7   Mon 17:30   H45

Machine learning for training lattice based models — •MATTIAS ÅNGQVIST, ERIK FRANSSON, J. MAGNUS RAHM, and PAUL ERHART — Chalmers University of Technology, Department of Physics, Gothenburg, Sweden

Creating lattice based models for studying configurational and vibrational effects has now become possible with little technical effort. The basic idea is that the models will be trained using reference data which commonly comes from expensive density functional theory calculations. If the training goes well the model will both accurately predict the training data but may also predict unseen data and do so at a fraction of the computational cost. The training is evaluated by cross validation by splitting up the reference data into testing and training sets. The number of optimization algorithms that one may choose to do the training with are very numerous. In this talk I will present how the different optimization algorithms perform when training these so called lattice based models both with respect to error estimation and to the prediction of e.g. thermodynamic quantities.

MM 10.8   Mon 17:45   H45

Reliable methods for combining tight binding models based on maximally localized Wannier functions — •JAE-MO LIHM and CHEOL-HWAN PARK — Department of Physics, Seoul National University, Seoul 08826, Korea

Maximally localized Wannier functions (MLWFs) form a set of localized orthogonal basis functions of a periodic system which accurately represent given Bloch states. [1] MLWFs are commonly used as building blocks for large-scale tight-binding calculations. For example, MLWFs generated from ab initio calculations on the bulk and a thin slab of a given material may be used to construct a tight-binding model for a thicker slab, or a semi-infinite slab. However, the corresponding MLWFs of different systems are not identical to their partners. This discrepancy may cause artifacts in the physical quantities calculated from the combined tight-binding model if not properly taken care of.

In this work, we propose two post-processing methods that correct the differences between the MLWFs in two different systems. First, we describe a minimal correction which is simple and efficient, but fails in complex systems. Next, we propose a more accurate and generally applicable correction method based on the hopping parameters. We demonstrate the utility of our correction methods by applying them to real materials. We also compare the corrected MLWFs with the Wannier functions constructed without maximal localization.

[1] N. Marzari et al., Rev. Mod. Phys. 84, 1419 (2012)

MM 10.9   Mon 18:00   H45

Phonon-Related Properties in Metal-Organic Frameworks from First Principles — •TOMAS KAMENCEK[1], SANDRO WIESER[1], EGBERT ZOJER[1], and NATALIA BEDOYA-MARTÍNEZ[1,2] — [1]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria — [2]Materials Center Leoben, Austria

Metal-organic frameworks (MOFs) are crystals consisting of metallic and organic constituents, which form open and porous structures. These materials have been extensively studied during the last years due to their numerous possible applications exploiting the large amount of internal surface area (e.g. catalysis, storage, capture and separation of gases). Phonon-related properties of MOFs, despite their importance for describing practically relevant quantities as thermal conductivity or thermal expansion, are still largely unexplored. Moreover, the huge number of building blocks and ways of connecting them to assemble a MOF opens the possibility to design materials with tailor-made properties. This calls for developing an in-depth understanding of phonons and phonon-related properties in MOFs. Therefore, we studied the influences of different constituents on the (an)harmonic phonon properties by means of atomistic simulations. Starting from MOF-5 we have systematically varied metallic nodes and organic linkers in order to deduce reliable structure-to -property relationships for phonon properties in MOFs. Our simulations have been performed in the framework of density functional tight binding theory with a focus on predicting elastic constants, phonon dispersions relations, and deduced quantities.

MM 10.10   Mon 18:15   H45

Phonon filters in molecular junctions — •ALVARO RODRIGUEZ MENDEZ[1,2], LEONARDO MEDRANO SANDONAS[1,2], RAFAEL GUTIERREZ[1], JESUS UGALDE[3], VLADIMIRO MUJICA[4], and GIANAURELIO CUNIBERTI[1,5] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [3]Kimika Fakultatea, Euskal Herriko Unibertsitatea (UPV/EHU) and Donostia International Physics Center (DIPC); P.K.1072; 20080 Donostia; Euskadi (Spain) — [4]Arizona State University, School of Molecular Sciences, Tempe, AZ 85287, USA. — [5]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden, Germany

We provide computational support to the intriguing idea that heterogeneous molecular junctions, consisting of molecular wires bridging two different nano-contacts, can act as a phonon filter. The filtering effect is ultimately due to the asymmetric nature of the contacts that translate into different interfacial energy transferring properties. The most important finding is the appearance of gaps on the phonon transmittance spectrum, which are strongly correlated to the properties of the vibrational spectrum of the molecule in the junction. This filtering effect may have very important technological implications for the design of smart nano-devices and nano-materials that can be used to control the asymmetric transmission of heat.

MM 10.11   Mon 18:30   H45

Phonon spectrum, phase stability and thermodynamic properties of the cubic pi-phase in the IV-VI monochalcogenides - formation and effect of a phonon band gap — •URI ARGAMAN, RAN ABUTBUL, and GUY MAKOV — Materials Engineering Department, Ben-Gurion University of the Negev, Beer Sheva 84105, Israel.

The pi phase is a recently discovered cubic phase in the IV-VI monochalcogenides with theoretical and technological interest (ref. 1). In this work, the phonon frequencies were calculated ab-initio in the cubic pi-phase of the monochalcogenides in four materials: SnS, SnSe, GeS and GeSe. All four were found to be mechanically stable, and a phonon band gap appears in their spectra. The phonon spectra of all these systems exhibit phonon band gaps in the optical phonon spectrum with widths of 0.7-2 THz. The origin of the phonon band gap was examined through an analysis of the normal modes. The contributions of the geometry of the bonds and mass differences to the phonon spectrum and, in particular, to the band gap are discussed and analyzed. We found differences in the relative motion of the two types of atoms and the rigidity of the bonds in this low symmetry structure. The effect of the phonon band gap on the thermodynamic properties is discussed. In addition, Raman experiment supported the existence of the phonon band gap in pi-SnS and pi-SnSe.

1. Abutbul, R. E., Segev, E., Argaman, U., Makov, G. and Golan, Y. (2018), Monochalcogenide Semiconductors: π*Phase Tin and Germanium Monochalcogenide Semiconductors: An Emerging Materials System. Adv. Mater., 30: 1870310. doi:10.1002/adma.201870310

MM 11: Symposium SYCO of the divisions MM (leading), O, CPP, KFM and DS continued as topical session: Mechanically controlled electrical conductivity of oxides (joint session MM/CPP/O)

Sessions: SYCO II and III

Time: Monday 15:45–18:30   Location: H46

Topical Talk   MM 11.1   Mon 15:45   H46
Probing the properties of dislocations in $SrTiO_3$ through transient transport measurements — •Roger De Souza — Institute of Physical Chemistry, RWTH Aachen University, 52056 Aachen, Germany

There is renewed interest in the interaction between oxygen vacancies and dislocations in the perovskite oxide $SrTiO_3$, driven by the material's possible application in devices for all-oxide electronics and for resistive switching. In my talk, I will demonstrate how transient transport experiments — comprising $^{18}O/^{16}O$ isotope exchanges and Secondary Ion Mass Spectrometry (SIMS) analysis — can be used to obtain a deeper understanding of this interaction. Having first introduced the thermodynamics of space-charge formation at extended defects, I will focus on describing experiments and simulations on various geometries: annealed single crystals, bicrystals, and polished single crystals. Finally, I will discuss how these studies allow us to arrive at a consistent description of point-defect behaviour at dislocations in $SrTiO_3$.

MM 11.2   Mon 16:15   H46
Characterization of Fe:STO thin films prepared by pulsed laser deposition — •Maximilian Morgenbesser, Stefanie Taibl, Markus Kubicek, Alexander Viernstein, Christopher Herzig, Andreas Limbeck, and Jürgen Fleig — TU Wien, Wien, Österreich

The perovskite-type oxide SrTiO3 (STO) is one of the best investigated materials in solid state ionics and commonly used as a model material in solid state ionics. The defect model of bulk SrTiO3 is well understood and the conductivity of bulk samples can be tailored by acceptor or donor doping, e.g. with Fe3+ or Nb5+ on the Ti4+ site. However, other aspects of SrTiO3 have not been understood so far, for example the the influence of factors such as stoichiometry and strain on the conductivity which is investigated in this study.

Two different kinds of 2 % Fe-doped thin films were deposited by pulsed laser deposition (PLD). Thin films deposited from stoichiometric targets exhibit a low, intrinsic conductivity. In addition, targets with Sr overstoichiometry were used and the conductivity could be increased by four orders of magnitude. The thin films are compared to each other in regard to the structure and stoichiometry. Structural differences could be found by x-ray diffraction measures, revealing a difference in lattice parameters. The chemical composition was analyzed by means of inductively coupled plasma optical emission spectroscopy (ICP-OES) and differences in the A/B ratios could be found. A model linking the conductivity to the stoichiometry of the thin films is presented, highlighting the possible impact of cation vacancies and antisite defects on the electrical conductivity of Fe:SrTiO3.

MM 11.3   Mon 16:30   H46
Generation of controlled dislocation structures in SrTiO3 and TiO2 for elucidating dislocation impact on electrical properties. — •Lukas Porz, Till Frömling, and Jürgen Rödel — Institute of Materials Science, Technische Universität Darmstadt, 64287 Darmstadt, Germany

Dislocations have been understood to alter numerous functional properties of ceramic materials, such as conductivity[Whitworth 1975]. Recently, modification of functional properties of oxide materials by dislocations receives much attention due to their various potentials for application[Szot 2018]. Especially the complex dislocation structure of naturally occurring dislocations makes investigations of dislocation effects difficult. Thus, disentangling the different effects of dislocations requires an ordered structure of the dislocations. So far ordered structures were primarily fabricated in bi-crystal interfaces which are often not comparable to natural dislocation arrangements.

We present a route to control the arrangement of the dislocations locally. Different slip systems can be individually introduced and an arrangement of all dislocations lying in the same set of slip planes was achieved. With identical line vectors, the dislocations connect two surfaces of a bulk sample which was shown by dark field x-ray microscopy. This well-arranged and well-understood structure of dislocations is a pre-requisite for unambiguous interpretations of detailed experiments on functional properties. The value of a controlled arrangement of dislocations is demonstrated by conductivity data along dislocation lines and across slip bands in comparison to a dislocation free reference.

45 min. break

MM 11.4   Mon 17:30   H46
Atomic and electronic structure of wurtzite ZnO(0001) inversion domain boundaries — •Jochen Rohrer and Karsten Albe — FG Materialmodellierung, FB Material- und Geowissenschaften, Technische Universität Darmstadt

In a recent work [1], variations of the conductivity of ZnO bicrystal samples with $(0001)||(0001)$ and $(000\bar{1})|(000\bar{1})$ orientations (inversion domain boundaries, IDB) due to the modulation of the potential barrier height at the IDB with respect to strain [2] has been demonstrated. In order to establish a more profound understanding of this behavior, a detailed characterization of the atomic structure and electronic properties of such IDBs by means of first-principles methods will be valuable. However, despite the structural and chemical variability of this system, only a few atomistic models have been in studied to date [3].

In this work we comprehensively study ZnO{0001} IDBs by means of density functional theory calculations. In particular, we construct a variety of structurally and chemically different phase-pure models and identify their thermodynamic stability within the allowed range of the O chemical potential. For stable models we investigate electronic properties and their response to strain. Finally we also study the role of various dopants, commonly added in experimental bicrystal samples.

[1] P. Keil *et al.*, *Adv. Mater.* **30**, 1705573 (2018). [2] D. R. Clarke, *J. Am. Ceram. Soc.* **82**, 485 (1999). [3] S. Li *et al.*, *Phys. Status Solidi B* **255**, 1700429 (2017).

MM 11.5   Mon 17:45   H46
Impact of internal electric field on the grain boundary barrier height of ZnO — •Bai-Xiang Xu, Ziqi Zhou, and Till Frömling — Institute of Materials Science, TU Darmstadt

Polycrystalline ZnO ceramics with grain boundary potential barriers are important materials for surge arresters due to their non-linear current-voltage behavior, and have potential application in advanced devices. Different grain boundary barrier height models have been developed by considering the direct piezoelectric effect. However, the piezoelectric charge should not only result from the direct piezoelectric effect, but also from the inverse piezoelectric effect, which refers to the mechanical response of the material by the electric field. Due to the charges at the grain boundary, strong internal electric field can be expected, and it leads to strain change through the inverse piezoelectric effect. This strain further modifies the polarization and thus leads to additional piezoelectric charges at the grain boundary and in the depletion layer. Thus, this should also be taken into account self-consistently. For this purpose we employ both analytical model and finite-element numerical simulation to reveal the impact of internal electric field on the GB barrier height and its stress sensitivity. Results show that the piezoelectric charge induced by the internal field tends to adjust the grain boundary charge and lowers the barrier height. Furthermore, the barrier height becomes less sensitive to mechanical stress and applied voltage if the influence of the internal field is taken into account. The extended model with the inverse piezoelectric effect of the internal field allows to further elucidate their piezotronic response.

MM 11.6   Mon 18:00   H46
Influence of cation order and strain on Na diffusion in $Na_3Zr_2Si_2PO_{12}$: A computational study — •Lisette Haarmann and Karsten Albe — Technische Universität Darmstadt, Otto-Berndt-Str. 3 64287 Darmstadt

$Na_3Zr_2Si_2PO_{12}$ is a solid electrolyte which is part of the Na super ionic conductor (NASICON) family. Experimentally, only Si/P lattice positions can be determined, but not the distribution of P on these sites[1]. This distribution, however, plays a crucial role for the Na diffusion. A systematic study of different cation orders is conducted using Molecular Dynamics (MD) simulations. Due to the strong correlation of diffusion in this material, the calculation of D_σ is necessary to obtain the ionic conductivity from the Nernst-Einstein equation[2]. By calculating D_σ and the tracer diffusion coefficient D_{tr}, Haven ratios are determined. Additionally, a jump rate model was developed, which allows investigation of correlation between individual jumps.

Moreover, it has been reported that doping can strongly increase the diffusivity of Na in NASICON materials[3]. In many cases, this is attributed to enlarged bottlenecks of diffusion. These doping elements, however, do not only contract or dilate the lattice structure but alter the chemical environment of the Na ions as well. In an effort to study purely the effect of mechanical deformation, the strain dependence of D_{tr} and the activation energy E_A is investigated.

[1] Boilot, J.P., *et. al.*, Journal of Solid State Chemistry **73**, (1988)
[2] Murch, G., Solid State Ionics **7**, (1982)
[3] Guin, M., Tietz, F., Journal of Power Sources **273**, (2015)

MM 11.7   Mon 18:15   H46
The impact of mechanical stresses on the ionic conductivity

of nanoparticles — •Peter Stein[1], Bai-Xiang Xu[1], and Karsten Albe[2] — [1]TU Darmstadt, FB 11, FG Mechanik funktionaler Materialien — [2]TU Darmstadt, FB 11, FG Materialmodellierung

Nanostructured electrodes have found wide application in electrochemical systems, for instance for lithium-ion batteries. This is due to their featuring short diffusion paths and large surface areas, allowing for comparatively fast surface reactions and transport within the slender bulk material. At this length-scale, surface stresses acting on the electrode surface induce a (non-uniform) pressure within the material, providing mechanical stabilization. As a result, nanostructured electrodes exhibit high reversible capacities and stable cycling behavior [1] as well as a higher robustness against mechanical degradation [2]. However, the surface-induced pressure field also affects the electrochemical behavior of the particle, modifying, among other things, surface reaction rates and ionic mobility.

In this contribution, we discuss the interaction of mechanical stresses with the electrochemical behavior of nanostructured electrode particles. We thereby consider ideal analytical shapes, faceted nanoparticles, and regular nanostructures such as inverse opal electrodes. We further demonstrate the impact of surface-stress-induced mechanical fields on defect thermodynamics and kinetics, chemical reactions, and phase transformations.

[1] N. Zhao et al., Pure Appl. Chem. 80:2283-2295, 2008. [2] C.K. Chan et al., Nat. Nanotechnol. 3:31-35, 2008.

MM 12: Poster session I

Time: Monday 19:15–20:45   Location: Poster C

MM 12.1   Mon 19:15   Poster C
Amorphous interlayers in semiconductor metallization —
•Dennis König, Efi Hadjixenophontos, Guido Schmitz, and Kevin Treder — Institute of Materials Sience, Chair of Material Physics, University of Stuttgart, Heisenbergstraße 3, 70569, Germany

Deposition of thin metallic films on monocrystalline silicon substrates has been extensively used in the past. An amorphous interlayer of few nm, between the silicon and the metallic coating is reported in such systems. During this work detailed investigation on this interlayer is done. Different parameters are studied such as: The cleaning time of the substrates, the power during deposition and the metallic element (Al, Au and Ag) in contact with the substrate. Samples are prepared by Ion beam sputtering with controlled thicknesses and are characterized by HRTEM after FIB cross sections. Further elemental analysis is done by EDX during microscopy. A clear dependency of the thickness of interlayer is observed on the cleaning time and power during deposition. Attempts to identify the composition of the amorphous interlayer are performed by Atom Probe Tomography.

MM 12.2   Mon 19:15   Poster C
Chemical bonding effects on the brittle-to-ductile transition in metallic glasses — •Franco Moitzi[1], Daniel Sopu[1,2], and Jürgen Eckert[1,3] — [1]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstrasse 12, 8700 Leoben, Austria — [2]Institut für Materialwissenschaft, Technische Universität Darmstadt, Otto-Berndt-Straße 3, 64287 Darmstadt, Germany — [3]Department Materials Physics, Montanuniversität Leoben, Jahnstraße 12, 8700, Leoben, Austria

By using molecular dynamics simulations we investigate the influences of composition and temperature on tensile deformation behavior of amorphous PdSi and CuZr alloys. While the plastic deformation in CuZr metallic glass occurs highly localized in one mature shear band, PdSi glass shows brittle cracking perpendicular to the loading direction. The crystal orbital hamilton population analysis based on electronic structure calculation from electronic structure calculation has revealed that the difference in the chemical bonding is responsible for the observed different deformation behaviors. The rigidity of the bonding impedes the strain and stress redistribution in PdSi metal-metalloid glasses and leads the brittle failure. Moreover, a brittle-to-ductile transition can be achieved upon increasing the temperature or/and decreasing the amount of silicon. The prevention of stress accumulation due to stress redistribution is identified to be the reason for the observed transition.

MM 12.3   Mon 19:15   Poster C

3D X-ray Diffraction Microscopy (3DXRD) using high resolution X-ray nanodiffraction — •Hergen Stieglitz[1], Christina Krywka[1], and Martin Müller[1,2] — [1]Helmholtz-Zentrum Geesthacht, Geesthacht, Deutschland — [2]Universität Kiel, Kiel, Deutschland

The existing technology called 3DXRD, is a well-established technique to map the grain structure of polycrystalline systems (e.g. metals). This technology is based on reconstruction algorithms which trace the positions of multiple Bragg-Peaks as a function of the rotation angle during the rotation of the sample. Due to a given beamsize and the software-based limit only a few grains can be tracked, resulting in a minimum mappable grainsize.

The planned experiment shall utilize a nano-focused synchrotron beam (e.g. Nanofocus Endstation of P03, PETRA III) to examine very fine-grained systems. The small beamsize allows detecting grains below the size limit of standard 3DXRD. With respect to the small beamsize of about 250 nm cross section, the precise positioning of the sample becomes more important to secure a constant scanned volume (the so called gauge volume). Otherwise some grains may be outside the gauge volume in some scans therefore they cannot be traced and produce mistakes while reconstructing.

To meet this challenge a stable and wobble-free rotary stage is planned to ensure a constant gauge volume. We are planning to use an interferomenter-based feedback loop to compensate the runout of the sample with a XY-stage.

MM 12.4   Mon 19:15   Poster C
Combining small-angle neutron scattering and analytical microscopy: An advanced method to characterize nano-precipitates in Ni-based superalloys — •Robert Lawitzki[1], Ralph Gilles[2], Michael Hofmann[2], Julia Wagner[1], and Guido Schmitz[1] — [1]Universität Stuttgart, IMW, Lehrstuhl für Materialphysik — [2]TU München, FRMII

We present an experimental method for the differentiation and quantification of the two strengthening phases, γ' and γ'', in the Ni-based superalloy Inconel 718. For this alloy, an individual quantification of those phases is experimentally very difficult and was, by now, only achieved by nano-scaled characterization techniques. In this contribution, we are applying the technique small-angle neutron scattering (SANS) on differently heat-treated specimens to individually quantify the nanoprecipitates in bulk average. The interpretation of the SANS signal required a structural model that could only be set up by complementary information that were obtained mainly by transmission electron microscopy (TEM) and atom probe tomography (APT). The advantage of using bulk neutron diffraction for quantification is that

several tens of cubic millimeters are analyzed and thus, significantly better statistics are obtained. The measured volume fractions of the γ"- precipitates are remarkably lower than stated in previous works, but now well fulfill the chemical mass balance. It will be further shown how this method can be adapted to other superalloys.

MM 12.5 Mon 19:15 Poster C

Real-time monitoring of laser powder bed fusion process using high-speed X-ray imaging — •Jan Rosigkeit[1], Dieter Lott[1], Marc-André Nielsen[1], Benjamin Wahlmann[2], Tao Sun[3], Marcus Rackel[1], Peter Staron[1], Florian Pyczak[1], and Martin Müller[1] — [1]Institute of Materials Research, Helmholtz-Zentrum Geesthacht, Germany — [2]Department of Materials Science and Engineering, University of Erlangen-Nuremberg, Germany — [3]Advanced Photon Source, Argonne National Laboratory, USA

We employ the high-speed synchrotron hard X-ray imaging technique to monitor the laser powder bed fusion process of Ti-6Al-4V powder on a Ti-42Al-8.5Nb-0.2C base plate in situ and in real time. Many scientifically and technologically significant phenomena in laser powder bed fusion, including melt pool dynamics, powder ejection, rapid solidification and keyhole pore formation are experimentally revealed with high spatial and temporal resolutions. The data present here will facilitate the understanding of dynamics and kinetics in metal laser powder bed fusion process.

The laser beam carrying various powers entered into the chamber straight down on the powder bed. The laser was operated in a spot-heating mode and in a line scanning mode. The X-ray beam impinged on the samples horizontally providing a side view of the powder bed.

All image series were taken with a frame rate of 50 kHz and an exposure time of 1 μs for each individual image. It can be observed that the process starts with the melting of theTi-6Al-4V powder around the laser spot and then the Ti-42Al-8.5Nb-0.2C base plate.

MM 12.6 Mon 19:15 Poster C

Status of the materials science x-ray scattering beamline BL9 of DELTA — •Michael Paulus, Christian Sternemann, and Metin Tolan — Fakultät Physik/DELTA, Technische Universität Dortmund, D-44221 Dortmund, Germany

Beamline BL9 is a multi-purpose x-ray scattering beamline at the synchrotron radiation facility DELTA located at the TU Dortmund, Dortmund, Germany. The beamline is dedicated to x-ray reflectivity, x-ray diffraction, small-angle x-ray scattering and fluorescence experiments using hard x-rays predominantly in the energy range between 10 keV and 30 keV. The current experimental setup will be presented and selected examples of prototype experiments will be given, ranging from investigations of biological to solid state samples as well as applications in cultural heritage. Future experimental perspectives will be discussed in light of the implementation of a new superconducting wiggler.

MM 12.7 Mon 19:15 Poster C

Deoxidation of copper surfaces by a dilectric barrier discharge plasma — •Aaron Arendt[1], Sebastian Dahle[1], and Wolfgang Maus-Friedrichs[1,2] — [1]Clausthaler Zentrum für Materialtechnik, TU Clausthal, Leibnizstr. 9, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany

The production in the metalworking industry takes place in the presence of oxygen. Although, attempts are made to keep the concentration of oxygen low with the aid of technical high vacuum and inert gases, there is still an oxide layer on the metal surfaces, which can form immediately under these conditions. This oxide layer could be advantageous for applications, for example in joining processes. State of the art is to reduce the surface by heat treatment with the help of high temperatures in order to make connections possible. Here, we present an alternative process in form of a DBE plasma in an argon/hydrogen atmosphere using the example of an oxidized copper sample. This plasma is used to reduce the copper oxide surface at room temperature. To reduce also deeper layers, the copper is additionally heated to allow diffusion processes to take place. X-ray photoelectron spectroscopy (XPS) is used to investigate the surface stoichiometry and depth profiling is done with a combination of sputtering and auger electron spectroscopy (AES). We show that 60 s of plasma treatment leads to an appreciable deoxidation of the copper surface.

MM 12.8 Mon 19:15 Poster C

The inline branch of the Swedish Materials Science Beamline P21.2 at PETRA III — •Timo Müller, Zoltan Hegedüs, Sven Gutschmidt, Thomas Bäcker, and Ulrich Lienert — Deutsches Elektronen-Synchrotron DESY, Photon Science, Hamburg, Germany

The high-energy beamline P21 at the third generation synchrotron source PETRA III is dedicated to materials science and is funded by Sweden. The instrumentation of the inline branch, P21.2, is designed to combine complementary experimental techniques (WAXS/SAXS/imaging) for the investigation of bulk samples and interfaces. The photon energy can be chosen in the range from 40 to 150 keV. The beam size can be varied from millimeters down to (sub-) microns by focusing with compound refractive lenses. This is the basis for the in-situ characterization of microstructures and phase transformations using various techniques, particularly during thermo-mechanical processing. The beamline has seen first light in September 2018 and is currently in its commissioning phase. First results will be presented and discussed. The goal is to give a comprehensive overview of the possibilities for future user experiments, since the beamline will start user operation in the second half of 2019.

MM 12.9 Mon 19:15 Poster C

the structural, thermodynamics, nonlinear properties and vibrational analysis of 4',5'-dibromo-2',7'-dinitro-3-oxo-3H-spiro[2-benzofuran-1,9'-xanthene]-3',6'-diolate — •Jean Baptiste Famkam Fankam[1], Jean Mari Bienvevu Ndjaka[1], and Jeh Wilson Geh[2] — [1]University of Yaounde I, Yaounde, Cameroon — [2]National Higher Polytechnic Institute, University of Bamenda, Bamenda, Cameroon

This review gives an overview concerning the structural, thermodynamics, nonlinear properties and Vibrational analysis of 4',5'-dibromo-2',7'-dinitro-3-oxo-3H-spiro[2-benzofuran-1,9'-xanthene]-3',6'-diolate which has been theoretically studied. We used the RHF and DFT (PBE1PBE, MPW1PW91, B3PW91 and B3LYP) approach to calculate the optimized parameters, Dipole moment **, average polarizability *α*, anisotropy ***, first hyperpolarizabilitiesβ, the zero-point vibrational energy ZPVE, sum of electronic energy without zero-point correction Eelec, with zero-point correction E0, with thermal energy E, with enthalpies H, with free energies G, contribution of thermal energy correction Ethermal, molar heat capacity at constant volume Cv and entropy S with cc-pVDZ basis set. In addition, we also computed IR and Raman activity spectrum. Our results suggest that this molecule have potential applications as linear and nonlinear optical materials. In spite of the large hyperpolarizability of this molecule, we are optimistic that this molecule has a potential application in the *eld of optoelectronic and medicine. This can be a promising material for optical limiting applications.

MM 12.10 Mon 19:15 Poster C

Analysis of the phase transition processes of sodium borohydride and first tests about its rehydration by means of cold dielectric barrier discharge plasmas — •Maik Szafarska[1,2], Georgia Sourkouni-Argirusi[1], and Wolfgang Maus-Friedrichs[1,2] — [1]Clausthaler Zentrum für Materialtechnik, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany

In the last decade, sodium borohydride has attracted attention in energy storage research, caused by its high hydrogen density and relatively low cost, making it a potentially better hydrogen (and energy) storage unit compared to compressed hydrogen gas tanks and liquid hydrogen. Therefore it would be an innovation for fuel cell economy and energy storage. To make it economically viable, its dehydration temperature has to be lowered and a new rehydration method has to be found. The phase transition mechanisms are a key for understanding the behavior of the material during these two processes. To investigate the phase transition and the rehydration of the material further, Thermogravimetric- and Multi Gas-Analysis were performed. The experimental results show that released hydrogen and the decomposition of the material occur during different phase transitions. Additionally first tests about the rehydration via dielectric barrier discharge plasmas show optimistic results.

MM 12.11 Mon 19:15 Poster C

Ab-initio Phase Stabilities of Ce-based Hard Magnetic Materials — •Halil ibrahim Sözen, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany

Due to the developments in e-mobility and renewable energies, hard

magnets composed of rare earths have gained increasing importance in the last decades. Recently, there is a growing interest in developing alternative hard magnetic materials, that reduce or even remove the need to use their expensive RE elements. The strategy is to use 3d elements with high magnetic anisotropy such as e.g. Fe-Co-B alloys. In order to support these efforts, we performed ab initio calculations of finite temperature phase stabilities of Ce-based alloys. The Helmholtz free energy F(T, V) is calculated for all relevant competing phases using a sophisticated set of methods capturing vibrational, electronic, magnetic and configurational entropy contributions. The study includes unary Ce, binaries of Ce-Fe and Fe-Ti phases, and ternary Ce-Fe-Ti phases. In a first step, we test the performance of our approach and find good agreement with experimental data. In a second step, we calculate the finite temperature phase formation diagram. This diagram shows that the presence of the CeFe2 phase prevents any formation of the targeted hard magnetic Ce-Fe-Ti alloys. This observation is supported by recent EDS experiments. In a third step, we, therefore, extend our study to quaternary alloys. Specifically, we study the effects of Cu and Ga substitution by introducing a screening scheme that allows testing all 3d and 4d elements.

MM 12.12   Mon 19:15   Poster C

Beyond the typical use of symmetry in Crystal structure prediction — •James Darby — TCM, Cavendish lab, University of Cambridge, UK

First-principles crystal structure prediction (CSP) is a well established technique which is routinely used to predict crystal structure in a diverse range of systems such as periodic solids, interfaces, encapsulated nanowires etc. However, one downside of CSP is that the number of minima in the potential energy surface scales exponentially with system size. As such, it rapidly becomes computationally unfeasible to search for more complex structures with larger unit cells. Here we discuss how going beyond the normal use of symmetry in CSP can be used to overcome this difficulty and work with more complex systems. In particular we focus on the generation of symmetric trial structures and how the distribution of these can lead to very biased searching if not done carefully. Results from structure searching using a modified version of the ab initio random search technique, and the CASTEP density functional theory code, will also be presented. In particular Magnesium Sulfide compounds will be discussed with reference to their use as anode materials in Magnesium ion batteries.

MM 12.13   Mon 19:15   Poster C

icet - A Pythonic approach to cluster expansions — •Mattias Ångqvist[1], William A. Muñoz[1], J. Magnus Rahm[1], Erik Fransson[1], Paul Erhart[1], Céline Durniak[2], Piotr Rozyczko[2], and Thomas Holm Rod[2] — [1]Chalmers University of Technology, Department of Physics, Gothenburg, Sweden — [2]Data Management and Software Centre, European Spallation Source, Copenhagen, Denmark

Many materials exhibit some form of chemical ordering, which can have a crucial impact on their macroscopic properties. Here, atomic scale modeling based on the so-called alloy cluster expansion (CE) technique can yield very valuable information. In this contribution, we present the open-source icet package that provides an efficient implementation of this methodology. It takes advantage of state-of-the-art machine learning techniques to generate accurate and predictive models based on quantum mechanical calculations. The icet package features a Python interface that enables seamless integration with other Python libraries including for example SciPy or scikit-learn. Yet, all computationally demanding parts are written in C++ providing performance while maintaining portability. We demonstrate the application of icet by (1) studying chemical ordering and associated properties in a series of intermetallic clathrates as a function of composition and temperature and (2) by predicting the phase diagrams of bulk and surface alloys.

MM 12.14   Mon 19:15   Poster C

Atomistic Simulation of Incipient Plasticity in Compressed Au Nanowires — •Aviral Vaid[1], Subin Lee[2], Julien Guenole[1], Arun Prakash[1], Sang Ho Oh[2], and Erik Bitzek[1] — [1]Materials Science and Engineering, Institute I, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — [2]Department of Energy Science, Sungkyunkwan University (SKKU), Suwon, Republic of Korea

Modern in-situ TEM experiments offer a unique possibility of imaging the nucleation of dislocations and the resulting plasticity in metallic nanowires. But the time resolution of these experiments is often too limited to study the details of dislocation-based deformation processes.

Here, we present our results on recent atomistic simulations addressing the mechanisms and conditions under which prismatic dislocation loops can form during uniaxial compression tests of [110] oriented Au nanowires as reported by Lee et. al (Nat. Comm., 2014, 5, 3033). Such dislocations with Burgers vector parallel to the compression axis were unexpected, as they experience no resolved shear stress during uniaxial compression. Molecular dynamics simulations using an EAM potential and different indenter types and radii as well as nanowire geometries and sizes allowed to reproduce the observed prismatic dislocation loops and identify their formation mechanism. Building a model based on the geometry of the nanowire cap and the indenter radius, we derived a criterion under which conditions prismatic loops could form. Furthermore, we deduced the size range of asperities on the nominally flat punch indenter necessary for the formation the prismatic dislocation loops observed in experiments.

MM 12.15   Mon 19:15   Poster C

Tuning the electronic structure of organometallic Kagome systems — •Marius Fuchs, Domenico Di Sante, and Giorgio Sangiovanni — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, D-97074 Würzburg

We investigate organometallic Kagome systems consisting of 2 metal ions coordinated by DCA organic groups. The system was predicted to exhibit characteristic Kagome bands close the the Fermi level as a result of tight binding-like interaction of 'superatomic' p-orbitals originating in the organic system[1]. Our investigation focuses on tuning the electronic structure of synthesizable[2] thin films along with constituent metal ions and possible doping. In that we give special attention to the Fermi surface and its potential instabilities at van-Hove filling.

[1] L. Z. Zhang et al. 2016, Intrinsic Two-Dimensional Organic Topological Insulators in Metal - Dicyanoanthracene Lattices, NanoLetters, 16, 2072 - 2075
[2] G. Pawin et al. 2008, A Surface Coordination Network Based on Substrate-Derived Metal Adatoms with Local Charge Excess, Angew. Chem. Int. Ed. 2008, 47, 8442 - 8445

MM 12.16   Mon 19:15   Poster C

Atomistic investigation of non-stoichiometric stacking faults in Fe-Nb alloys — •Ali Zendegani[1], Michaela Šlapáková Poková[1,2], Christian Liebscher[1], Frank Stein[1], Sharvan Kumar[3], Thomas Hammerschmidt[4], Fritz Körmann[1], Tilmann Hickel[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Charles University, Prague, Czech Republic — [3]Brown University, Providence, USA — [4]Ruhr-Universität Bochum, Bochum, Germany

In Fe-Nb alloys a hardening via tetrahedrally close-packed (TCP) phases (e.g. Laves Fe$_2$Nb and μ Fe$_7$Nb$_6$) can be achieved. At the same time, various types of stacking faults occur during deformation. To investigate the correlation of both features in a Nb-rich Laves phase, *ab initio* calculations are combined with thermodynamics concepts.

By performing gamma surface calculations we resolve the atomic structure of these planar faults and show that they have a surprising geometrical complexity. Introducing a new thermodynamic framework allows us to compare the stability of planar faults (2D) with bulk phases (3D) in a convex hull diagram. The resulting diagram reveals that Nb-rich crystal structures next to basal and pyramidal stacking faults can become energetically more favorable than the nucleation of an epitaxially constrained μ phase. Excess Nb results thus in an enhanced formation of 2D stacking faults rather than forming 3D Nb rich precipitates in form of the μ phase. This unexpected finding allows a direct interpretation of recent HR-TEM studies on this materials system.

MM 12.17   Mon 19:15   Poster C

A first-principle self-consistent phonon approach for studying the vibrational properties of the high-temperature phases of pervoskites. — •Sohaib Ehsan, Marco Arrigoni, Georg Madsen, and Peter Blaha — Institute of Materials Chemistry, Vienna University of Technology, Vienna, Austria

In this study we investigate the phonon properties of perovskites in their high-temperature phases by first- principle methods. We use BaTiO3 , which shows a stable cubic phase above 120 C, as a model material. Due to the presence of unstable phonon modes in the harmonic approximation, we include an-harmonicity by calculating self-consistently temperature-dependent interatomic force constants. We show that in this way we are able to reproduce the experimentally ob-

served phonon dispersion relations. Such approach allows to predict other vibrational properties of these compounds, such as the transition temperature between the low- and high-symmetry phases and the lattice thermal conductivity.

MM 12.18   Mon 19:15   Poster C

The AiiDA-KKR plugin for high-throughput ab-initio impurity embedding — ●Fabian Bertoldo, Philipp Rüssmann, Jens Bröder, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We present the AiiDA-KKR package [1,2] which enables users to conveniently perform complex tasks with the JuKKR package through AiiDA [3] (Automated interactive infrastructure and database for material science). Therefore, the plugin and its respective workflows are introduced. They significantly reduce the workload of the user by automating most of the trivial steps of large-scale scientific calculations. Especially, results will be stored in a database and the provenance of all conducted steps (inputs, checkpoints, results) can be tracked and accessed at any desired point. The workflows and calculation can be launched with simple python scripts. Using this framework, we calculate the behavior of impurities in different host systems. Due to the high-throughput design of AiiDA and the AiiDA-KKR package we are now able to investigate multiple of those impurities in an easy manner which was not possible before by just using the plain KKR code.
[1] https://github.com/JuDFTteam/aiida-kkr
[2] https://aiida-kkr.readthedocs.io
[3] G. Pizzi, et al. Comp. Mat. Sci. 111, 218-230 (2016)

MM 12.19   Mon 19:15   Poster C

Mixing thermodynamics of MoO_3–WO_3 solid solutions from first-principles calculations — ●Jongmin Yun[1], Ricardo Grau-Crespo[2], and Aloysius Soon[1] — [1]Department of Materials Science & Engineering, Yonsei University, Seoul 03722, Korea — [2]Department of Chemistry, University of Reading, Reading RG6 6AD, United Kingdom

To date, solid solutions of high work-function transition metal oxides, e.g., MoO_3 and WO_3 are still poorly understood due to the complexity of site-occupancy disorder in these solid solution systems. Having a deeper understanding of these oxide solid solution systems will greatly benefit the engineering of new oxide heterojunction devices. Here, we perform first-principles density-functional theory calculations for the $(MoO_3)_x(WO_3)_{1-x}$ solid solution and multi–configurational supercell analysis for the reliable mixing thermodynamics. Namely, we aim to report the relative thermodynamic stability of these solid solutions as a function of mixing ratios with regards to the parent polymorphic phases. Moreover, we examine the trends in the electronic structure of the energetically favored configurations.

MM 12.20   Mon 19:15   Poster C

pyiron - an integrated development environment (IDE) for computational material science — ●Jan Janssen[1], Sudarsan Surendralal[1], Osamu Waseda[1], Liam Huber[1], Yury Lysogorskiy[2], and Joerg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Bochum, Germany

The past years witnessed tremendous progress in computational materials science both with respect to predictive power and scalability (e.g. high-throughput computations). These advances are not only related to the large gain in computer power but often to the development of advanced and computationally highly efficient algorithms and methods. A challenge in this respect is that the resulting simulation protocols are getting ever more complex: They often require the combination of high performance codes implemented in low-level programming languages with incompatible input/output formats, the implementation of flexible interfaces to dynamically adjust the order of the tasks in the simulation protocol, and the distribution of tasks on highly heterogeneous computing platforms. To foster the development of these novel techniques and their dissemination and use in our department we started several years ago with the development of the pyiron integrated development environment (http://pyiron.org). This framework allows to automatise routine tasks, to automatically store input/output data of all the individual jobs in a generic format together with the simulation protocols and the parent-child relationship of the tasks.

MM 12.21   Mon 19:15   Poster C

Computational study of the electronic properties of electrode materials — ●Janis K. Eckhardt[1,2], Markus S. Friedrich[1,2], Simon Burkhardt[1,2], Michael Czerner[2,4], Matthias T. Elm[1,2,3], Christian Heiliger[2,4], and Peter J. Klar[1,2] — [1]Institut of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen, Germany — [2]Center for Materials Research (LaMa), Heinrich-Buff-Ring 16, 35392 Giessen, Germany — [3]Institute of Physical Chemistry, Heinrich-Buff-Ring 17, 35392 Giessen, Germany — [4]Institute for Theoretical Physics, Heinrich-Buff-Ring 16, 35392 Giessen

Lithium ion batteries are widely used as power sources in portable electrical applications. In particular with regard to the optimization of existing applications or the development of new technologies, it is necessary to understand the fundamentals of ionic and electronic transport inside the active cathode material. Most scientists are examining cathode materials by using composite electrodes which also contain additives influencing their electrochemical properties. In order to avoid such influences, it is desirable to investigate the electrochemical properties of the pure active material. By performing density functional theory calculations, especially, with focus on equimolar lithium nickel cobalt manganese oxide (NCM-111), it was possible to gather additional information about its electronic structure. The screened Korringa-Kohn-Rostoker method has been employed in these calculations. Density of states calculations with reference to $Li_{1-x}[Ni_{1/3}Co_{1/3}Mn_{1/3}]O_2$ for different amounts of lithium within the crystal structure imply changes of the magnetic moment of the transition metals.

MM 12.22   Mon 19:15   Poster C

Smart-data machine learning for surface polymorph search — ●Andreas Jeindl, Lukas Hörmann, Alexander T. Egger, and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

The major challenge of surface structure search is the large number of possible polymorphs. The SAMPLE approach [1,2] can help circumvent this problem. It combines a coarse-grained potential energy surface with Bayesian linear regression to efficiently predict the adsorption energies of an exhaustive set of commensurate organic monolayers.

In this contribution we present the SAMPLE approach. The first step is finding all local minima for a single molecule on the surface. We then create all possible combinations of these local minima up to a certain unit cell size. With the help of 'experimental design' theory, we select a subset of maximally diverse structures. This subset is evaluated with dispersion-corrected density functional theory and used as training set for a Bayesian linear regression model. The linear regression uses an energy model based on the assumption that the main interactions on the surface are governed by molecule-substrate interactions and pairwise molecule-molecule interactions. Thus, we can not only predict the adsorption energies of millions of possible polymorphs, but also gain meaningful physical insight.

We use three complementary molecules on coinage metals to showcase the capabilities of our approach.
[1] Scherbela et al., Phys. Rev. Materials 2, 043803
[2] Hörmann et al., arXiv:1811.11702

MM 12.23   Mon 19:15   Poster C

DFT study of the charge density wave metal LuNiC2 — ●Soner Steiner[1,2,3], Herwig Michor[2], and Dominik Legut[1] — [1]IT4Innovations, VSB - Technical University of Ostrava, Ostrava, Czech Republic — [2]Institute of Solid State Physics, TU Wien, 1040 Wien, Austria — [3]University of Applied Sciences Wiener Neustadt, Austria

We have investigated the charge density wave (CDW) metal LuNiC2 by means of density functional theory (DFT) . We report on the electronic structure, fermi surface and the CDW transition. The formation of a significant gap due to the CDW transition is seen in the density of states at the Fermi level, which reduces the electronic density of states from N(Ef)=1.03 states/eV f.u. without CDW to N(Ef)=0.4 states/eV f.u. . The Sommerfeld value corresponding to the CDW density of states at the Fermi level is in reasonable agreement with the experimental value. The formation of the CDW modulated structure is causing a fragmentation of the Fermi surface into several isolated electron and hole pockets.

MM 12.24   Mon 19:15   Poster C

A first-principles study of the phase diagram of solid hydrogen — ●Alice Shipley, John Trail, and Richard Needs — Cavendish Laboratory, University of Cambridge, UK

Hydrogen is the most abundant element in the universe and the simplest atom. However, the behaviour of dense hydrogen is far from simple. Solid hydrogen possesses a rich phase diagram and, as a substance predicted to exhibit room-temperature superconductivity at high pressures [PRL 21, 1748 (1968)], has been of experimental and theoretical interest for decades. In computational studies, density functional theory (DFT) traditionally offers an attractive balance between accuracy and cost; a consideration which is essential here as there are many candidate structures separated by static-lattice enthalpy differences on the order of meV/atom. It is therefore also essential to consider vibrational effects in order to determine phase stability. Unfortunately, the solid hydrogen phase diagrams produced using different standard exchange-correlation functionals do not qualitatively agree with one another. With this in mind, our work explores the accuracy of purpose-built exchange-correlation functionals for high-pressure hydrogen [PRB 95, 115116 (2017)]. The new pressure-temperature phase diagrams obtained will be presented alongside a discussion of the vibrational self-consistent field (VSCF) approach [PRB 87, 144302 (2013)] used to incorporate vibrational effects, including anharmonicity.

MM 12.25 Mon 19:15 Poster C

Hydrogen detection in high strength steels with Scanning Kelvin Probe Force Microscopy — •Ines Traxler[1,2], Gabriela Schimo-Aichhorn[1], Andreas Muhr[3], Gerald Luckeneder[3], Hubert Duchaczek[3], Karl-Heinz Stellnberger[3], Josef Faderl[3], Darya Rudomilova[4], Tomáš Prošek[4], and Sabine Hild[1,2] — [1]CEST Competence Center for Electrochemical Surface Technology, Viktor-Kaplan Str. 2, 2700 Wr. Neustadt and Stahlstr. 2-4, 4031 Linz, Austria — [2]Institute of Polymer Science, Johannes Kepler University, Altenbergerstr. 69, 4040 Linz, Austria — [3]voestalpine Stahl GmbH, voestalpine-Str. 3, 4020 Linz, Austria — [4]UCT Prague, Zizkova 7, 27801 Kralupy, Czech Republic

Hydrogen embrittlement is a big problem in the automotive industry, as even small amounts of hydrogen have detrimental effects on steel properties. Scanning Kelvin Probe Force Microscopy (SKPFM) is a hopeful technique for the investigation of hydrogen in steel and the visualization in the individual steel phases with a very good spatial resolution. The impact of hydrogen diffusion on zinc coated high strength steels was investigated using SKPFM. Also, the hydrogen insertion at cut edges and coating defects was studied. To induce corrosion and to promote hydrogen entry into steel, various salt solutions were applied on the backside of uncoated and zinc coated dual phase steels. The hydrogen inserted into the sample is subsequently permeating through the steel until it reaches the other sample side,where the effect on the contact potential difference (CPD) and therefore the hydrogen permeation is monitored with SKPFM.

MM 12.26 Mon 19:15 Poster C

AuCuNiPdPt as a benchmark for high entropy alloys — •Jens Freudenberger[1,2], Felix Thiel[1,3], Alexander Kauffmann[4], Martin Heilmaier[4], and Kornelius Nielsch[1,3] — [1]IFW Dresden — [2]TU Bergakademie Freiberg — [3]TU Dresden — [4]Karlsruhe Institut für Technologie

The high entropy alloy AuCuNiPdPt appears single-phase and with the Cu-type structure. Additionally, non-stoichiometric alloys made from any of these elements with arbitary composition also crystallise single-phase with the Cu-type structure. Therefore, these alloys can be used to separate the material behaviour of the HEAs cleanly from that of single phase conventional alloys and to identify which issues are special for HEAs leading to their peculiar properties. The present study presents the mechanical behaviour and a microstructure analysis of AuCuNiPdPt.

MM 12.27 Mon 19:15 Poster C

Characterization of diffusive transport in polycrystalline tungsten trioxide thin films — •Jan L. Dornseifer[1,2], Alexander G. Strack[1,2], Simon Burkhardt[1,2], Matthias T. Elm[1,2,3], and Peter J. Klar[1,2] — [1]Institute of Experimental Physics I, Justus-Liebig-Universität, Germany — [2]Center for Materials Research (LaMa), Justus-Liebig-Universität, Germany — [3]Institute of Physical Chemistry, Justus-Liebig-Universität, Germany

Tungsten trioxide (WO_3) is an electrochromic material, thus, it can change its optical properties through insertion of charge carriers. Its electrochromic properties depend on the deposition process and resulting morphology. Polycrystalline WO_3 thin films are prepared by electron-beam evaporation and a subsequent heat treatment at $450\,°C$. To investigate the diffusive transport of hydrogen in WO_3, the elec-

trochemical properties are estimated by measurments using the galvanostatic intermittent titration technique (GITT) and electrochemical impedance spectroscopy (EIS). The impedance spectra obtained are fitted with a Randles circuit. The self-bleaching of WO_3 influences the experimental data in a significant way which has an impact on the evaluation of the data and the determination of the diffusion coefficients. In situ transmission measurements during the impedance spectroscopy reveals an oscillating behavior of the transmission at excitation signal frequencies below $91\,mHz$. This interesting behavior may yield additional information about the diffusive ion transport.

MM 12.28 Mon 19:15 Poster C

Impact of Severe Plastic Deformation on Al_xCoCrFeNi High Entropy Alloys — •Lena Frommeyer[1], Mehdi Eizadjou[2], Anna Ceguerra[2], Peter K. Liaw[3], Harald Rösner[1], Sergiy Divinski[1], Simon Ringer[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Australian Center for Microscopy and Microanalysis, University of Sydney, Australia — [3]Department of Materials Science and Engineering, The University of Tennessee, Knoxville, TN 37996, USA

During the last few years, a new class of materials called high entropy alloys has been extensively studied. The multi-principal element approach opens a wide compositional space with complex possibilities of combining 5 or more elements, each of them having originally equiatomic concentration. The main research focus was initially set to obtain single-phase alloys. However, secondary phases in alloys can lead to improved properties. In this study, the high entropy alloy Al-CoCrFeNi was modified by adding Al in various amounts. Moreover, the arc melted and homogenized alloys have been severely deformed by high pressure torsion (HPT). Subsequently, the un-deformed as well as the severely deformed alloys were examined by X-ray diffraction, electron back-scatter diffraction/transmission Kikuchi diffraction, transmission electron microscopy, energy-dispersive X-ray spectroscopy and atom probe tomography. Transitions from pure fcc to fcc+B2 and to fcc+B2+A2 as well as severe grain refinement and high twin densities were observed and are discussed with respect to the variations of composition and strain.

MM 12.29 Mon 19:15 Poster C

Magnetic properties of the CoCrFeMnNi high entropy alloy — •Soner Steiner[1,2,3], Sergii Khmelevskyi[4], and Dominik Legut[1] — [1]IT4Innovations, VSB - Technical University of Ostrava, Ostrava, Czech Republic — [2]Institute of Solid State Physics, TU Wien, 1040 Wien, Austria — [3]University of Applied Sciences Wiener Neustadt, Austria — [4]Center for Computational Materials Science, Vienna University of Technology, Wiedner Hauptstrasse 8, 1040 Vienna, Austria

We investigated the elastic properties and magnetism of the high entropy alloy CoCrFeMnNi in the basis of first principles. We have calculated the elastic properties at elevated temperatures taking into account longitudinal spin fluctuations (LSF). We show that LSF essentially renormalize the elastic constants compared to those calculated for magnetically ordered state. With the use of calculated exchange constants in paramagnetic state we attempt to understand the kind of magnetic ordering in this system. We also employ the locally self-consistent Green's function (LSGF) within the exact muffin tin method (ELSGF) formalism to visualize the random spin glass like state by performing the first-principles calculations for large random supercells (up to 500 atoms).

MM 12.30 Mon 19:15 Poster C

Experimental Studies of Helium Diffusion and Trapping in Tungsten — •Vassily Vadimovitch Burwitz[1,2,3], Thomas Schwarz-Selinger[2], Thomas Dürbeck[2], Georg Holzner[2,4], Rodrigo Arrendo Parra[2,4], and Christoph Hugenschmidt[1,3] — [1]Physik Department E21, TU München — [2]Max-Planck-Institut für Plasmaphysik (IPP) — [3]Heinz Maier-Leibnitz Zentrum (MLZ) — [4]Lehrstuhl für Plasma-Material-Wechselwirkung, Fakultät für Maschinenwesen, Technische Universität München, 85748 Garching, Germany

Helium is insoluble and highly mobile in tungsten. However, bubbles and blisters are commonly found in helium ion exposed samples. While the bubble growth parameters are known, the bubble nucleation process is still unclear. A hypothesized explanation based on ab initio calculations is a combination of self-trapping and trap mutation. Three independent experimental methods are used to check these predictions: Temperature Programmed Desorption (TPD), Elastic Recoil Detection Analysis (ERDA) and Coincident Doppler Broadening

Spectroscopy (CDBS). In combination, these techniques will yield trap concentration, trap energy, and helium distribution. A unique TPD setup that can reach a maximum temperature of 3000 K while preserving UHV conditions, a CDBS setup located at the worlds brightest positron source (NEPOMUC) and a foil-ERDA setup as well as first measurements of the system He in W will be presented.

MM 12.31   Mon 19:15   Poster C
Determination of the Vacancy Formation Enthalpy of La by Positron Annihilation Spectroscopy — •Lucian Mathes, Thomas Gigl, and Christoph Hugenschmidt — Heinz Maier-Leibnitz Zentrum (MLZ) and Physik Department E21, Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

The coincident Doppler broadening (CDB) spectrometer at the positron beam facility NEPOMUC of the FRM II enables spatially resolved defect studies by using Doppler broadening spectroscopy (DBS) of the positron-electron annihilation line. In order to perform depth dependent measurements of the near-surface region and the bulk of a sample, the positron implantation energy can be set up to 30 keV. A heatable sample holder enables temperature dependent in-situ defect spectroscopy from room temperature up to 1000 K. By using temperature dependent DBS we succeeded in determining the vacancy formation enthalpy of La for the first time. First, the as-received samples were annealed in situ, i.e. the decrease of the so called S-parameter indicated the annealing of lattice defects. For comparison, Cu served as reference material. During a second heating cycle the increase of the vacancy concentration was clearly observed which allowed a calculation of the vacancy formation enthalpy. In addition, a temperature dependence of the vacancy formation enthalpy in La was observed. Financial support by BMBF (project no. 05K10WOB) is gratefully acknowledged.

MM 12.32   Mon 19:15   Poster C
Grain-boundary diffusion in CoCrFeNi and CoCrFeMnNi high entropy alloy polycrystals — •Marcel Glienke[1], Mayur Vaidya[1], Lukasz Rogalc[2], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Westfälische-Wilhelms Universität, Institut für Materialphysik, Münster, Deutschland — [2]2Institute of Metallurgy and Materials Science, Polish Academy of Sciences, 30-059 Krakow, Poland

For the first time, grain boundary (GB) diffusion of Co, Cr, Fe and Mn have been measured in polycrystalline CoCrFeNi and CoCrFeMnNi high entropy alloys (HEAs) using the radiotracer technique. The alloys have been prepared using high frequency electromagnetic induction melting followed by homogenization at 1200°C for 50 h. X-ray diffraction confirms the single phase FCC structure of both the HEAs. Scanning electron microscopy along with electron back-scattered diffraction (EBSD) validates the equiatomic composition and coarse grained microstructures. Radioactive isotopes 57Co, 51Cr, 59Fe and 54Mn have been utilized to measure grain boundary self-diffusion in the temperature range of 800°C - 1000°C. The temperature and time of diffusion annealing are selected to ensure the B-type kinetics conditions for both the HEAs. The temperature dependence of the GB diffusion coefficients follows Arrhenius behavior for all the constituents in the HEAs. The obtained results are compared on the homologous temperature scale with GB self-diffusivities in other FCC matrices.

MM 12.33   Mon 19:15   Poster C
invar effects in FeNiCo medium entropy alloys: from an invar treasure map to alloy design — •ziyuan rao[1], dirk ponge[1], fritz körmann[1,2], yuji ikeda[1], oldřich schneeweiss[3], martin friak[3], jörg neugebauer[1], dierk raabe[1], and zhiming li[1] — [1]Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [2]Materials Science and Engineering, Delft University of Technology, 2628 CD Delft, The Netherlands — [3]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, v.v.i., žižkova 22, Brno CZ-616 62, Czech Republic

To facilitate the understanding and design of FeNiCo-base invar alloys characterized by low thermal expansion coefficient (TEC), we investigated the magnetic and thermal expansion behavior of an equiatomic prototype medium entropy alloy FeNiCo and a non-equiatomic (super invar) Fe63Ni32Co5 (at. %) reference alloy by means of experiments and ab initio calculations. Large spontaneous volume magnetostriction is observed in both alloys below their respective Curie temperatures. The invar effect in the non-equiatomic Fe63Ni32Co5 alloy is of step-type with nearly zero TEC over a wide temperature range (from room temperature to 120 oC) below its Curie temperature. The relationships among magnetic behavior, spontaneous volume magnetostriction and

invar effects for a wider array of metallic alloys are discussed based on Masumoto*s rule and Wohlfarth*s itinerant electron theory. An invar alloy search map is constructed based on the present results and available literature data, which provides a design route for further developments of new invar alloys by tuning their magnetic properties.

MM 12.34   Mon 19:15   Poster C
atomic mobilities of fcc Co-V-Mo alloys: measurement and modeling — •Jingfeng Zhang[1], Yong Du[2], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, Westfälische-Wilhelms University of Münster, Münster, Germany — [2]State Key Laboratory of Powder Metallurgy, Central South University, Changsha, China

Co is widely used as a matrix binder phase for cemented carbides. Certain addition of V and Mo in Co can minimize the grain size of cemented carbides, behaving as the grain growth inhibitors. Though diffusion plays a key role in material manufacturing process, there are no investigations of diffusion kinetics of this ternary system so far.

Based on 18 sets of diffusion couples, the composition-dependent interdiffusion coefficients in the fcc Co-rich Co-V-Mo alloys at 1273, 1373 and 1473 K were obtained from the intersection points of the diffusion couples by means of EPMA technique coupled with the Whittle and Green method. With the experimentally determined interdiffusion coefficients and the critically reviewed experimental diffusivities available in the literature, the atomic mobilities of fcc Co-V-Mo alloys were assessed using Diffusion Controlled Transformation (DICTRA) software. The quality of the assessed atomic mobilities was confirmed by the comprehensive comparisons between various DICTRA-calculated diffusion behaviors and the experimental ones, including concentration profiles and diffusion paths. The results will be critically examined against direct measurements of the tracer diffusivities by the radiotracer technique.

MM 12.35   Mon 19:15   Poster C
Grain-boundary diffusion in CoCrFeNi and CoCrFeMnNi high entropy alloybi-crystals — •Alexandra Everwand[1], Daniel Gaertner[1], Bengü Tas[1], Yury Chumlyakov[2], Gerhard Wilde[1], and Sergiy V. Divinski[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Department of Physics of Metals, Tomsk State University, Tomsk, Russia.

The diffusion kinetics in the equiatomic quaternary CoCrFeNi and quinary CoCrFeMnNi high entropy alloys, the so-called Cantor-alloys, were previously investigated using the radiotracer technique in single- and poly-crystalline materials. For the first time, diffusion of all constituent elements and additionally solute diffusion of Mn in the quaternary alloy is investigated in bi-crystalline HEAs with a defined grain-boundary. In order to define the microstructure, the chemical composition of the bi-crystals and the grain-boundary structure, scanning electron microscopy (SEM), electron back-scatter diffraction (EBSD), energy dispersive X-ray spectroscopy (EDX) and transmission electron microscopy (TEM) analyses are performed. Using the radiotracer technique, the grainboundary diffusion coefficients of 57Co, 51Cr, 59Fe, 54Mn and 63Ni are determined at a temperature of 1373 K according to Harrison's B-type, and at a temperature of 923 K according to Harrisons's C-type. The components are characterized by significantly different diffusion rates, with Mn being the fastest element and Ni and Co being the slowest ones.

MM 12.36   Mon 19:15   Poster C
Brute force composition scanning with a CALPHAD database to find low temperature bcc high entropy alloys — •Peter Klaver, Darko Simonovic, and Marcel Sluiter — Department of Materials Science and Engineering, Delft University of Technology, Mekelweg 2, 2628CD Delft, The Netherlands

We used Thermo-Calc CALPHAD calculations to determine the stable phases of AlCrMnNbTiV, AlCrMoNbTiV, AlCrFeTiV and AlCrMnMoTi alloys. A five- or six-dimensional grid is constructed, with stable phases calculated at each grid point. Three million compositions were calculated, resulting in ~20000 compositions consisting of a single disordered bcc phase down to 800 K. By filtering out compositions with a single disordered phase, composition islands of high entropy alloys are determined. The sizes and shapes of such islands provide information about which element combinations have good high entropy alloy forming qualities as well as about the role of individual elements within an alloy. We determined which compositions lie near the centers of these islands and thus remain high entropy islands under small composition changes. These compositions make good candidates for experimental

verification. The search for high entropy islands can be conducted under constraints, e. g. requiring a minimum amount of Al and/or Cr to promote oxidation resistance. It is also possible to look for alloys consisting of two different disordered phases. The high entropy forming qualities of AlCrMnNbTiV and AlCrMoNbTiV are relatively good, those of AlCrFeTiV are poor, while those of AlCrMnMoTi are poor at 800 K but quickly become better with increasing temperature.

MM 12.37   Mon 19:15   Poster C
Universal 1/f type current noise of Ag filaments in redox-based memristive nanojunctions — •Botond Sánta[1,2], Zoltán Balogh[1,2], Ágnes Gubicza[1,3], László Pósa[1,4], Dávid Krisztián[1], György Mihály[1,2], Miklós Csontos[1,3], and András Halbritter[1,2] — [1]Department of Physics, Budapest University of Technology and Economics, Budapest, Hungary — [2]MTA-BME Condensed Matter Research Group, Budapest, Hungary — [3]Empa, Swiss Federal Laboratories for Materials Science and Technology, Trans-

port at Nanoscale Interfaces Laboratory, Dübendorf, Switzerland — [4]Institute for Technical Physics and Materials Science, Centre for Energy Research, Hungarian Academy of Sciences, Budapest, Hungary

The microscopic origins and technological impact of 1/f type current fluctuations in Ag based, filamentary type resistive switching devices have been investigated. The analysis of the low-frequency current noise spectra revealed that the main electronic noise contribution arises from the resistance fluctuations due to internal dynamical defects of the Ag nanofilaments. The resulting 0.01-1% current noise ratio is found to be universal: it only depends on the total resistance of the device, irrespectively of the material aspects of the surrounding solid electrolyte as well as of the specific filament formation procedure. Moreover, the resistance dependence of the current noise ratio also displays the diffusive to ballistic crossover, confirming that stable resistive switching operation utilizing Ag nanofilaments is not compromised even in truly atomic scale junctions by technologically impeding noise levels.

MM 13: Invited talk Langhammer

Time: Tuesday 9:30–10:00   Location: H43

Invited Talk   MM 13.1   Tue 9:30   H43
Single Nanoparticle Insights to Create the Fastest Hydrogen Sensor in the World — •Christoph Langhammer — Department of Physics, Chalmers University of Technology, SE-41296 Göteborg, Sweden

Metal nanoparticles exhibit localized surface plasmon resonance, which provides unique opportunities for optical sensing and for fundamental studies of individual nano-entities. For example, using plasmonic nanoparticles as signal transducers in a hydrogen sensor offers the ultimate miniaturization limit of the single nanoparticle. At the same time, being able to address individual nanoparticles upon interaction

with hydrogen gas opens up unique opportunities to investigate metal-hydrogen interactions at the fundamental level beyond the traditional ensemble-averaged response, and thus shed light on the role of nanoparticle size, shape and microstructure on both hydrogenation thermodynamics and kinetics.

In this talk, I will discuss the single nanoparticle nanoplasmonic hydrogen sensing concept from both perspectives outlined above. Specifically, I will outline the critical role of both grain boundaries and nanoparticle shape on the hydride formation kinetics and thermodynamics in Pd and Pd-alloy nanoparticles, as identified in single particle experiments, and how these findings provide fundamental design rules for the development of the fastest hydrogen sensor in the world.

MM 14: Topical session (Symposium MM): High entropy and compositionally complex alloys

Sessions: Properties II and Diffusion

Time: Tuesday 10:15–13:15   Location: H43

Topical Talk   MM 14.1   Tue 10:15   H43
Nanocrystalline high-entropy alloys studied by atomistic computer simulations — Daniel Utt, Leonie Koch, Alexander Stukowski, and •Karsten Albe — TU Darmstadt, FB 11, FG Materialmodellierung, Otto-Berndt-Str. 3, D-64287 Darmstadt

The superior mechanical properties of high-entropy alloys (HEA) can be mainly attributed to the fact that multiple principle elements tend to strengthen materials markedly by the solid-solution hardening mechanism. Randomly distributed elements in grain interiors can, however, also affect relative grain-boundary energies and minimize thermodynamic driving forces for grain- boundary migration. Moroever, segregation may occur at grain boundaries and work as barriers to prevent grain-boundary motion. These effects become particular imporant in the small grain-size regime. In this contribution results from combined molecular dynamics and Monte-Carlo simulations for a four-component model alloy are presented, which were carried out using an embedded-atom approach and an average potential method. After discussing the impact of local disorder on phonons and stacking fault energies, we present results on the structure and mobility of grain boundaries in bicrystal geometry and compare to result obtained from polycrytalline model structures. The simulations provide no evidence for a change in migration mechanisms, but show the influence of GB segregation and secondary phase formation. Furthermore, samples are studied under mechanical load and deformation mechanisms -in particular twin formation- are investigated.

MM 14.2   Tue 10:45   H43
Quinary TWIP-TRIP high-entropy alloys: design, microstructure and mechanical properties — •Xiaoxiang Wu, Yuji Ikeda, Fritz Körmann, Dierk Raabe, and Zhiming Li — Max-Planck-Institut für Eisenforschung,Düsseldorf,Germany
Quinary FeMnNiCoCr HEAs have shown great potential in obtain-

ing excellent combination of strength and ductility. By adjusting the atomic ratios of the five principal elements to reach appropriately low stacking fault energy (SFE), twinning-induced plasticity (TWIP) and/or transformation-induced plasticity (TRIP) effects can be introduced in the non-equiatomic quinary FeMnNiCoCr HEAs, leading to enhanced strength, ductility and working hardening capacity compared to the equiatomic HEA. In the present work, we combine ab initio calculation and experimental investigation to design various non-equiatomic quinary $Fe_{60-x-y}Mn_xNi_yCo20Cr20$ (at.%) HEAs. Three typical HEA compositions with comparably low SFE were chosen and alloys were then prepared and characterized. The results show that enhanced work hardening has been achieved by changing Ni concentration from 11 at.% to 6 at.% in the probed HEA system. In spite of the similar SFE level, the three HEAs under investigation demonstrate different primary deformation modes, changing from TRIP-dominant (with considerable TWIP), complete TWIP to TWIP-dominant (with negligible TRIP). The influences of SFE and the individual elements on the deformation modes are discussed to provide new insights into the further design of quinary TWIP-TRIP HEAs.

MM 14.3   Tue 11:00   H43
Strengthening in solid solutions of the system Au-Cu-Ni-Pd-Pt — •Felix Thiel[1,2], Christina Bollnow[1,2], Jens Freudenberger[1,3], David Geissler[1], Alexander Kauffmann[4], Hans Chen[4], Martin Heilmaier[4], and Kornelius Nielsch[1,2] — [1]IFW Dresden, Helmholtzstr. 20, 01069 Dresden — [2]TU Dresden, Institut für Werkstoffwissenschaft, Helmholtzstr. 7, 01069 Dresden — [3]TU Bergakademie Freiberg, Institut für Werkstoffwissenschaft, Gustav-Zeuner-Str. 5, 09599 Freiberg — [4]KIT, Institut für Angewandte Materialien - Werkstoffkunde, Engelbert-Arnold-Str. 4, 76131 Karlsruhe

High Entropy Alloys (HEAs) show outstanding mechanical and physi-

cal properties, which would not have been expected upon their simple crystal structure and the fact that they are single phased. The Au-Cu-Ni-Pd-Pt system and their including subsystems show crystallization into the same Cu-type crystal structure within the whole concentration range. Therefore,this system is unique and particularly suitable to study the alloying effect on the properties within a large concentration range without the necessity of considering other phases. The present study shows the effect of alloying a multi-component solid solution on the properties of medium and high entropy alloys in this system. In particular, effects such as solid solution hardening and work hardening are assessed.

MM 14.4 Tue 11:15 H43

abnormal magnetic behavior of FeNiCoMnCu high entropy alloys — •ZIYUAN RAO[1], ZHIMING LI[1], FRITZ KÖRMANN[1,2], BISWANATH DUTTA[2], DIRK PONGE[1], LUKAS SCHÄFER[3], KONSTANTIN SKOKOV[3], OLIVER GUTFLEISCH[3], and DIERK RAABE[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [2]Materials Science and Engineering, Delft University of Technology, 2628 CD Delft, The Netherlands — [3]Institut für Materialwissenschaft, Technische Universität Darmstadt, Darmstadt, Germany

In this project experimental and theoretical calculations are combined to unveil an abnormal magnetic behavior caused by the addition of nonmagnetic element Cu in face-centered cubic FeNiCoMn-based high entropy alloys (HEAs). We found that saturation magnetization of the as-cast HEAs at room temperature increases by 77% and 177% at Cu contents of 11 at. % and 25 at. %, respectively, compared to the equiatomic FeNiCoMn HEA without Cu addition. For HEAs homogenized at 1273 K for 2 h and water-quenched, the magnetic state transforms from paramagnetism to ferromagnetism at room temperature after 25 at. % Cu addition. For homogenized HEAs, ab initio calculations reveal an increase of Curie temperature caused by Cu addition and agree well with experimental results. By coupling the experimental and theoretic results, we unveiled the mechanisms responsible for the Cu effect on the magnetic properties of FeNiCoMn HEAs, which is fundamentally different from that reported in conventional binary or ternary alloys.

15 min. break

Topical Talk   MM 14.5 Tue 11:45 H43
Bulk and grain boundary diffusion in high entropy alloys — •MAYUR VAIDYA, SANDIPAN SEN, DANIEL GARTNER, GERHARD WILDE, and SERGIY DIVINSKI — Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

An intriguing aspect of High entropy alloys (HEAs) is their diffusion behaviour and there is yet a lack of consensus on the factors governing atomic transport rates in HEAs. The present talk attempts to provide a critical analysis of the diffusion measurements reported so far for HEAs and gives glimpses of current diffusion studies being performed at the research lab of University of Münster. The anticipated *sluggish* diffusion is clearly absent in FCC CoCrFeNi and CoCrFeMnNi HEAs, both in the lattice and along grain boundaries. Ni is slowest diffusing species in both the HEAs, while Mn diffusion is fastest in the quinary HEA. The diffusion rates are lower (by maximum an order of magnitude) in these HEAs when compared to lower component alloys only when a homologous temperature scale is used for the comparison. Diffusivity measurements in single crystals of these HEAs have hinted towards a possible contribution of dislocations to the penetration profile. The preliminary results of solute diffusion in HCP HEAs are also presented.

MM 14.6 Tue 12:15 H43

Radiotracer diffusion in single crystalline CoCrFeNi and CoCrFeMnNihigh entropy alloys — •DANIEL GAERTNER[1], JOSUA KOTTKE[1], YURY CHUMLYAKOV[2], GERHARD WILDE[1], and SERGIY V. DIVINSKI[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Department of Physics of Metals, Tomsk State University, Tomsk, Russia.

High entropy alloys are multicomponent alloys, which consist of five or more elements in equiatomic or nearly equiatomic concentrations. These materials are hypothesized to show significantly decreased self-diffusivities. For the first time, diffusion of all constituent elements in equiatomic CoCrFeNi and CoCrFeMnNi single crystals and additionally solute diffusion of Mn in the quaternary alloy is investigated using the radiotracer technique, thereby the tracer diffusion coefficients of

^{57}Co, ^{51}Cr, ^{59}Fe, ^{54}Mn and ^{63}Ni are determined in a temperature range between 923 K and 1373 K. The components are characterized by significantly different diffusion rates, with Mn being the fastest element and Ni and Co being the slowest ones in the quinary composition. In the quaternary composition Mn and Cr are the slowest elements at low temperatures and the situation is reversed with increasing temperature. Furthermore, solute diffusion of Cu in the CoCrFeNi single crystal is investigated in the temperature range of $973 - 1173$ K using the ^{64}Cu isotope. In the quaternary alloy, Cu is found to be a fast diffuser at the moderate temperatures below 1273 K and its diffusion rate follows an Arrhenius law with an activation enthalpy of about 149 kJ/mol.

MM 14.7 Tue 12:30 H43

Heat capacity, defect annihilation and tracer diffusion in the Ni–CoCrFeMn system: transition from a dilute solid solution to a high entropy alloy — •JOSUA KOTTKE[1], JONAS LÜBKE[1], ADNAN FAREED[1], DANIEL GAERTNER[1], MATHILDE LAURENT-BROCQ[2], LOÏC PERRIÈRE[2], ŁUKASZ ROGAL[3], SERGIY V. DIVINSKI[1], and GERHARD WILDE[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Université Paris Est, ICMPE (UMR 7182), CNRS, UPEC, F-94320, Thiais, France — [3]Institute of Metallurgy and Materials Science of the Polish Academy of Sciences, 30-059 Krakow, Poland

High-entropy alloys, i.e. multicomponent alloys with a large number of constituting elements in equiatomic or nearly equiatomic composition, attract an increased attention as potential structural materials due to their favorable physical and mechanical properties, especially at elevated temperatures. Here, we report on the changes in thermodynamic and kinetic properties regarding the transition from a dilute solid solution to a high entropy alloy.

The true heat capacity and tracer diffusion of all elements are measured in $Co_{20}Cr_{20}Fe_{20}Mn_{20}Ni_{20}$, $Co_{10}Cr_{10}Fe_{10}Mn_{10}Ni_{60}$ and $Co_2Cr_2Fe_2Mn_2Ni_{92}$ and compared to those in pure Ni. Furthermore, the annihilation of deformation-induced vacancies and the recrystallisation kinetics are investigated using differential scanning calorimetry. While tracer diffusion does not reveal any abrupt transition, the defect evolution and the microstructural response are shown to be distinct in the $Co_{10}Cr_{10}Fe_{10}Mn_{10}Ni_{60}$ alloy.

MM 14.8 Tue 12:45 H43

Solute diffusion in HCP high entropy alloys — •SANDIPAN SEN[1], MAYUR VAIDYA[1], LUKASZ ROGAL[2], BLAZEJ GRABOWSKI[3], SANKARAN SHANMUGAM[1,4], GERHARD WILDE[1], and SERGIY DIVINSKI[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Institute of Metallurgy and Materials Science of the Polish Academy of Sciences, 30-059 Krakow, Poland — [3]Max-Planck-Institut für Eisenforschung GmbH D-40237 Düsseldorf, Germany — [4]Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai-600036, India

Diffusion studies in high entropy alloys are still scarce and practically limited to FCC systems. For the first time, diffusion in HCP high entropy alloys is investigated using a radiotracer technique. Diffusion of Co (the so-called ultra-fast diffuser in α-Ti) is systematically measured in HfZr, HfZrTi, and Al-Hf-Sc-Ti-Zr alloys in the temperature range between 400°C - 800°C and, thus, the impact of the number of constituting elements on solute diffusion is examined. Two quinary systems (Al15Hf20Sc10Ti20Zr20 and Al5Hf20Sc20Ti20Zr20) are studied to elucidate the influence of the Al addition and of a possible short-range ordering on ultra-fast diffusion. The phase composition of the alloys was characterized by X-ray diffraction and transmission electron microscopy. The temperature dependence of the diffusion coefficients of Co is shown to follow Arrhenius behavior for all the alloys. The obtained results are compared on the homologous temperature scale with the solute diffusivities in other HCP matrices.

MM 14.9 Tue 13:00 H43

Microstructure and diffusion behavior of pseudobinary multicomponent intermetallic compounds — •MOHAN MURALIKRISHNA GARLAPATI[1,2], MAYUR VAIDYA[2], GERHARD WILDE[2], KAUSTUBH N. KULKARNI[3], SERGIY DIVINSKI[2], and MURTY B.S.[1] — [1]Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai 600036, India — [2]Institute of Materials Physics, University of Muenster, Muenster 48149, Germany — [3]Indian Institute of Technology Kanpur, Kalyanpur, U.P. 208 016, India

The current study investigates the possible formation of ordered B2 intermetallic compounds with the addition of multiple elements. In order to have the advantage of a light weight and high strength, a novel pseudo binary approach has been employed for alloy synthesis from binary to quinary. In each alloy, Al content is maintained as 50 at.% and other elements (Co, Fe, Mn and Ni) constitute the remaining 50 at.%. The alloys have been processed using vacuum arc melting followed by suction casting. Synthesized alloys have been homogenized at 1100° C for 5 days. X-ray diffraction analysis confirms the presence of B2 phase in all the alloys. Scanning electron microscopy validates a uniform phase composition and coarse grain microstructure. Self-diffusivities of the constituent elements in each of the alloys have been determined at 1100° C using radiotracer technique. Diffusion coefficients have been measured using tracer penetration profiles and are compared with literature and the impact of multi-element matrix on diffusion is discussed.

MM 15: Topical session (Symposium MM): Correlative and in-situ Microscopy in Materials Research

Sessions: Soft Matter and Hybrid Materials; Energy Materials

Time: Tuesday 10:15–13:15   Location: H44

Topical Talk   MM 15.1   Tue 10:15   H44
Correlative Microscopy of Biological Cells and Tissues by Scanning X-ray Diffraction, Holography, Tomography and Super-Resolution Optical Microscopy — Marten Bernhardt[1], Jan-David Nicolas[1], Andrew Wittmeier[1], Michael Sprung[1], Sarah Köster[2], and •Tim Salditt[1] — [1]Georg-August-Universität Göttingen — [2]DESY, Hamburg

We present a correlative microscopy approach , which combines holographic x-ray imaging, x-ray scanning diffraction, and super-resolution optical fluorescence microscopy, in particular stimulated emission depletion (STED)-microscopy [1], implemented in the same synchrotron endstation. This allows us to image both labeled and unlabeled molecular components in biophysical and soft matter samples in a quasi-simultaneous scheme. We exploit the complementary contrast mechanisms of x-ray microscopy and optical fluorescence for studies of heart muscle cells: While scanning x-ray diffraction and x-ray holographic imaging provide structural information on the native electron-density distribution within the cell, fluorescent markers visualize specific molecular components.

[1] M. Bernhardt, J.-D. Nicolas, M. Osterhoff, H. Mittelstädt, M. Reuss, B. Harke, A. Wittmeier, M. Sprung, S. Köster, T. Salditt. Nature Communications 9: 3641 (2018)

Topical Talk   MM 15.2   Tue 10:45   H44
Experimental observations of molecular ordering in slitconfined non-polar fluids — •Oliver H. Seeck, Milena Lippmann, Anita Ehnes, and Florian Bertram — Deutsches Elektronen-Synchrotron DESY, Notkestrasse 85, 22607 Hamburg, Germany

The molecular order of non–polar liquids constrained in slit–geometry of a few molecular diameters exhibits distinct features which cannot be found in bulk liquids. A well–known example is the formation of molecular layering along the surface normal of the confining substrates. Another aspect is the observation that the shear modulus and the viscosity of confined liquids are similar to those observed in the solid bulk phase. The latter phenomenon is known as confinement–induced solidification. Imaging the confined liquid films with Å–resolution in all tree dimenions is a greate challenge. We have developed a setup for film thicknesses down to 30 Å and which is compatible with X–ray scattering methods such as reflectivity, grazing incidence diffraction and Bragg-scattering. At confined CCl_4–films we have proven the co–existance of a layered phase and a crystalline phase. In the future we will investigate the response of the molecular order to shear forces being applied to the confined films with a new setup.

MM 15.3   Tue 11:15   H44
Establishing a mechanistic model for the synthesis of noble metal nanoparticles — •Tobias Zech[1], Tilo Schmutzler[1], Dennis Noll[1], Klaus Götz[1], Erdmann Spiecker[2], and Tobias Unruh[1] — [1]LKS, Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]CENEM, Friedrich-Alexander-Universität Erlangen-Nürnberg

In our research we are stuying in the interaction between gold nanorods (AuNRs) and the stabilizer in form of CTAB, and how the latter influences the morphology of AuNR during the synthesis. AuNRs have the potential to be integral parts in nanoplasmonic devices and in medicine as biomarker and for photothermal therapy. However, lacking reproducibility and low yield make the synthesis expensive. Additionally, CTAB, assumed to strongly adsorb to gold nanoparticles, makes it difficult to functionalize the surface. We use a combination of SANS and SAXS to analyze the behavior of CTAB micelles, gold nanoparticles and their CTAB stabilization layer in-situ. From this we want to develop a mechanistic model, which more accurately describes the anisotropic growth of AuNR. So far, we were able to develop a stabilization model for small gold nanoparticles with CTAB micelles and improve their long-time stability considerably. Furthermore, we could directly correlate the changes of the structure of CTAB micelles to the resulting aspect ratio of AuNRs, when certain additives are present. SAS experiments will play a vital role in developing deeper understanding of the underlying mechanisms of AuNR growth.

15 min. break

Topical Talk   MM 15.4   Tue 11:45   H44
In-situ Studies of Electrochemical Interfaces in Lithium-ion Batteries — •Hans-Georg Steinrück — SSRL Materials Science Division, SLAC National Accelerator Laboratory, Menlo Park, California 94025, USA

In lithium-ion batteries (LIBs), the arrangement of electrolyte molecules directly at the electrode interface, and the electric double layer (EDL) formation are expected to govern the interfacial ion transport during charge/discharge and the electrochemical stability, i.e. the origin and properties of the solid electrolyte interphase (SEI). The SEI is formed on anode surfaces due to electrolyte decomposition at low potentials outside the electrolyte's electrochemical stability window, and dictates cell chemistry, cycle life, and electrochemical reversibility.

Towards this end, the first topic of this talk discusses an Å-resolution combined experimental and theoretical structural determination of solid-liquid interfaces relevant to LIBs, specifically a baseline organic electrolyte containing various concentrations of lithium hexafluorophosphate salt at a metal oxide interface. The second portion of this talk describes a multi-property characterization study of the physical and chemical properties as well as the nucleation and growth of the SEI on silicon anodes relevant to LIBs. We combined in-situ X-ray reflectivity, linear sweep voltammetry, ex-situ X-ray photoelectron spectroscopy, and first principles calculations to develop a holistic understanding of the SEI formation mechanism and properties on native oxide terminated single crystalline Si electrodes.

MM 15.5   Tue 12:15   H44
Nanoscale Characterization of Energy Materials using SIMS based Correlative Microscopy — •Santhana Eswara, Alisa Pshenova, Jean-Nicolas Audinot, and Tom Wirtz — Advanced Instrumentation for Ion Nano-Analytics, MRT, Luxembourg Institute of Science and Technology, L-4422 Belvaux, Luxembourg

Energy materials play a key role in providing sustainable and eco-friendly energy solutions. To improve the efficiency of energy conversion and storage, modern materials are being increasingly designed at the nanoscale and the chemical compositions are tuned even down to the dopant level. Therefore, nanoscale high-sensitivity chemical analyses are required for (i) establishing the link between local nanoscale characteristics of the material and the overall device performance and (ii) to develop new strategies to enhance performance and improve durability. Our research on this subject is focused on addressing the associated analytical challenges. While Transmission Electron Microscopy (TEM) offers high spatial resolution, the conventional analytical techniques available in TEM are inadequate for the analysis of

light elements (H, B, Li) and dopant-level concentrations. Secondary Ion Mass Spectrometry (SIMS) offers high-sensitivity and all elements can be analyzed, but, the lateral resolution is fundamentally limited by ion-solid interaction volume to ~ 10 nm. To overcome this limitation, we use correlative TEM-SIMS [1] to investigate (i) silicon solar cell materials and (ii) electrodes in lithium battery materials. The results, correlative workflow, data treatment methods and potential artefacts will be discussed. [1] L. Yedra et al, Sci. Rep. 6, 28705, 2016

MM 15.6   Tue 12:30   H44
Dislocations in Cu(In,Ga)Se$_2$ solar cell absorbers: Insights from electron microscopy and electronic structure calculations — Daniel Barragan-Yani[1], Ekin Simsek Sanli[2], and •Karsten Albe[1] — [1]TU Darmstadt, FB 11, FG Materialmodellierung, Otto-Berndt-Str. 3, 64287 Darmstadt — [2]Max Planck Institute for Solid State Research, Stuttgart Center for Electron Microscopy, Heisenbergstrasse 1, 70569 Stuttgart

In Cu(In,Ga)Se$_2$ (CIGSe) based devices, power-conversion efficiencies of more than 15 % can be achieved, although significant dislocation densities are present. This still unexplained behavior is in contrast to what has been reported for other semiconductor materials, where the presence of dislocations strongly affects the electrical properties. This implies that lattice dislocations in CIGSe-based absorbers are per se electrically inactive or possibly passivated by solute or impurity atoms. In this contribution, calculations based on density functional theory are presented. which reveal the influence of chemical reconstruction and solute segregation on the activity of mixed and partial dislocations in CIGGe. The role of mechanical driving forces for point defect dislocation interaction is highlighted, which allows to explain results obtained from by aberration-corrected scanning transmission electron microscopy in combination with electron energy-loss spectroscopy.

MM 15.7   Tue 12:45   H44
Structural Characterization of the 2D-Powder Material DRCN5T:PC71BM Using X-rays — •Marvin Berlinghof[1], Stefan Langner[1], Christina Harreiss[1], Ella M. Schmidt[1], Rita Siris[2], Florian Bertram[3], Johannes Will[1], Stefanie Rechberger[1], Georg S. Duesberg[2], Reinhard B. Neder[1], Erdmann Spiecker[1], Christoph J. Brabec[1], and Tobias Unruh[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Deutschland — [2]Universität der Bundeswehr München, Neubiberg, Deutschland — [3]Deutsches Elektronen-Synchrotron, Hamburg, Deutschland

The crystallinity and with it the power conversion efficiency (PCE) of organic photovoltaic thin films made of small molecule-fullerene-blends is tune-able by solvent vapor annealing (SVA). An example of such a system are thin films of DRCN5T:PC71BM. The small molecule DRCN5T crystallizes during annealing with vapors of chloroform, tetrahydrofuran or carbon disulfide. Its crystallites are formed at the surface of the thin film as a 2D powder (oblique crystal system). In the crystallites, DRCN5T assembles itself in stacks, which form the 2D crystalline structure.

A comparison of in- and ex-situ grazing wide angle X-ray scattering (GIWAXS), X-ray pole figures, elastic electron diffraction, and secondary ion mass spectrometry (SIMS) measurements will be presented. This includes information about, the crystalline structure, preferred orientations, and the vertical composition of the photoactive layer.

MM 15.8   Tue 13:00   H44
Post-treatment processes and their effects on organic solar cell morphology and performance — •Christina Harreiss[1], Stefan Langner[2], Stefanie Rechberger[1], Johannes Will[1], Christoph J. Brabec[2], and Erdmann Spiecker[1] — [1]Institute of Micro- and Nanostructure Research & Center for Nanoanalysis and Electron Microscopy, Friedrich-Alexander Universität Erlangen-Nürnberg — [2]Institute of Materials for Electronics and Energy Technology, Friedrich-Alexander Universität Erlangen-Nürnberg

During the past decades the efficiency of solution-processed organic solar cells (OSCs) could be improved by developing new processing conditions. Since the morphology of OSCs determines the charge separation at the interfaces and the electron and hole transport to the electrodes, it influences the device performance. Analytical Transmission Electron Microscopy (TEM) techniques like energy filtered TEM (EFTEM) are used to study the morpholgy since conventional imaging techniques are mostly insufficient to visualize the donor and acceptor. Here we present results on a OSC system composed of a small molecule (DRCN5T) and a fullerene derivative (PC70BM). The active layers were treated by thermal annealing (TA) and solvent vapor annealing (SVA). The SVA was performed with different solvents and for different annealing times. The morphology was revealed for all post-treated active layers by EFTEM and correlated to the performance. Currently we are performing the TA directly in our TEM device by an in situ heating technique. By this, we can observe the phase separation and formation of an interpenetrating network of donor/acceptor phases.

MM 16: Methods in Computational Materials Modelling (methodological aspects, numerics)

Sessions: Nucleation; Interfaces

Time: Tuesday 10:15–13:15   Location: H45

MM 16.1   Tue 10:15   H45
Atomistic mechanism of nucleation in Ni: the role of pre-structuring and seeding in polymorph selection — •Grisell Díaz Leines and Jutta Rogal — Ruhr-Universität Bochum, Universitätsstrasse 150, 44780 Bochum, Germany

Understanding the fundamental principles of polymorph selection during crystal nucleation is essential in the control and prediction of materials properties. However, to obtain a precise knowledge of the crystallization mechanism is often challenging as most physical systems exhibit polymorphic transitions and are often heterogeneously seeded by the presence of impurities. Here we employ transition path sampling together with maximum likelihood estimation to analyze the atomistic mechanism of crystal nucleation in Ni. We further investigate the effect of small pre-structured seeds on the crystallization process. The analysis of the transition path ensemble reveals that the pre-structured liquid region that surrounds the nucleus plays a crucial role in the description of the nucleation process together with the amount of fcc particles in the core of the crystal cluster. Consistent with our interpretation of the nucleation mechanism, we demonstrate that seeds with structures compatible with those observed in the growing nucleus (fcc and pre-structured liquid) facilitate the nucleation and determine the polymorph selected, while seeds with hcp and icosahedral structures have neither an effect on the nucleation rate nor on the mechanism. Our results shed light on the atomistic processes of polymorph selection during crystallization in Ni.

MM 16.2   Tue 10:30   H45
Transition path sampling of homogeneous nucleation during solidification in molybdenum — •Sarath Menon, Grisell Díaz Leines, Jutta Rogal, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum

The investigation of nucleation during solidification on an atomic scale is challenging for both experimental and theoretical methods due to the involved time and length scales. Since nucleation time scales are many orders of magnitude larger than the ones achieved by classical molecular dynamics, we employ transition path sampling, an atomistic simulation method that generates an ensemble of dynamical trajectories between the liquid and the solid state. From the path ensemble, thermodynamic and kinetic properties such as the free energy barrier and the nucleation rate are calculated. We study homogeneous nucleation in Mo at various undercoolings and compare the effect of the interatomic potential on the calculated properties. Furthermore, we employ transition path sampling for analysis of the nucleation mechanisms by studying the polymorphs that are generated during the initial stages of nucleation and growth. The crystal core originates in a region of pre-ordered liquid, with BCC being the most abundant phase throughout nucleation. We further compare the nucleation mechanisms in molybdenum and nickel to reveal that the final bulk structure emerges at an early stage of nucleation.

MM 16.3   Tue 10:45   H45

Hysteretic phase transitions of IrTe2: a unified picture from ab initio approaches — •Gabriele Saleh and Sergey Artyukhin — Istituto Italiano di Tecnologia, Via Morego 30, Genova 16163 Italy

A number of metal dichalcogenides are promising candidates for cutting-edge applications [1]. IrTe2 displays peculiar temperature-induced phase transitions to phases with Ir-Ir dimers [2] that can be tuned by doping and triggered by photoexcitation [3]. These transitions display hysteresis and they are accompanied by a change in the physical properties of the material, thus opening possibilities for technological applications. The various phases differ by the length of certain Ir-Ir and Te-Te bonds, that change up to 25% [3]. While a wealth of experimental results exist, the atomic-level understanding of transitions in IrTe2 is still poor. Here we present an in-depth computational investigation of the electronic structure and lattice dynamics of IrTe2. We demonstrate, through the combined use of several chemical bonding analysis approaches, that the electronic stability of low-T phases is determined by the formation of Ir2Te2 4-centre bonds. The high-T phase, instead, is stabilized by the higher entropic contribution of its phonons. We rationalize the observed hysteresis by analyzing the energetics of phase transitions through the Nudged Elastic Bands method. Finally, we present our preliminary results on the effect of doping on both the band structures and the phonon spectra of the IrTe2 phases. REFERENCES: [1] C. Tan et al. , Adv. Mater., 29(37), 1701392 (2017). [2] Q. Li et al. , Nat. Comm., 5, 5358 (2014). [3] S. I. Ideta et al. , Sci. Adv., 4(7), eaar3867 (2018).

MM 16.4   Tue 11:00   H45

Atomistic Modelling of Early Stage Clusters In Al-Mg-Si alloys — •David Kleiven[1] and Jaakko Akola[1,2] — [1]Norwegian University of Science and Technology, Trondheim, Norway — [2]School of Chemical Technology, Aalto University, Aalto, Finland

Aluminium alloys are essential in a variety of industrial applications, including cars and aeroplanes. The mechanical properties, such as hardness and strength, depend heavily on the formation of beneficial precipitates from solute species. Interestingly, the precipitation process (and prior nucleation) can be manipulated via thermomechanical treatment. We apply the Cluster Expansion formalism as implemented in CLEASE (CLuster Expansioin in ASE) to construct a DFT-parametrised energy model for Al-Mg-Si alloys, which we further apply in finite temperature statistical simulations. Even though Al-Mg-Si is a common industrial alloy, the mechanisms behind the precipitation process are still not fully understood. In this contribution, the stable phases on the FCC lattice, which are important intermediates for needle-like precipitates, are identified with high accuracy (~5 meV/atom). We assess the role of various effects such as solute ordering and direction-dependent surface tension of solute clusters. Via this approach we obtain quantitative results for the thermodynamics of early stage clusters in Al-Mg-Si alloys which paves way for understanding the precipitation process at atomistic level.

MM 16.5   Tue 11:15   H45

Atomistic Study of Nucleation and Growth in Ni3Al — •Yanyan Liang, Grisell Díaz Leines, Jutta Rogal, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum

The initial stages of nucleation and growth are a crucial step during solidification. Atomistic insight into nucleation, in particular for binary alloys, still remains elusive due to the extended timescales and the complexity of the process. In this study, we focus on the binary alloy Ni3Al which is a key component in high-temperature superalloys. We employ transition path sampling to generate an ensemble of molecular dynamics trajectories, from which we extract thermodynamic and kinetic properties of the nucleation process. For Ni3Al, we obtain two different nucleation pathways that resemble the competition between two distinct bulk crystal structures, face-centred cubic and body-centred cubic. The size of the critical nucleus commonly used as reaction coordinate strongly depends on the structural composition and is therefore not sufficient to describe the nucleation in this binary system. Both the size and crystal structure of the growing nucleus need to be explicitly taken into consideration as reaction coordinates. Furthermore, we observe that the competition between diffusion and interface growth velocities has a decisive impact on the chemical order. In Ni3Al, the growth velocity surpasses the diffusion even for small undercooling of 1% which leads to disorder trapping with partial chemical order.

15 min. break

MM 16.6   Tue 11:45   H45

Machine learning and the thermodynamics of grain boundary segregation — •Liam Huber, Raheleh Hadian, Blazej Grabowski, and Joerg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Solute-grain boundary (GB) interaction critically impacts the evolution and stabilization of grain structure and thus has a strong impact on the final material properties. At the atomic scale, structural disorder at the GB can create a wide variety of local environments for segregating atoms, and thus a wide distribution of segregation energies. Using classical molecular statics, we perform high-throughput calculations of six solutes to 38 different boundaries in Al obtaining 1.4 million segregation energies. With this rich dataset, we demonstrate that the traditional Langmuir-McLean model, which approximates solute-GB interaction with a single effective energy, is insufficient. By applying machine learning techniques, we provide a new and computationally highly efficient path to obtain the full energy distribution of the solvents. Extending this approach we have also calculated a corresponding set of surface segregation energies. Using a similar distribution-based approach provides us with a direct route to assess the role of solutes on GB embrittlement.

MM 16.7   Tue 12:00   H45

Development of a layer-specific surface segregation model based on atomistic simulations beyond McLean — Tamara Krauss and •Sebastian Eich — Institut für Materialwissenschaft, Lehrstuhl für Materialphysik, Universität Stuttgart, Deutschland

In this atomistic study, layer-specific segregation to the surface is investigated for an exemplary (100) surface in iron–chromium alloys. Segregation is simulated in the semi-grand canonical ensemble using a thermodynamically accurate iron–chromium embedded-atom potential[1]. Through a continuous variation of the chemical potentials, the full composition range is explored in the temperature range from 400 K to 1400 K, enabling the analysis of surface segregation below and above the critical temperature of the miscibility gap. Taking the surface tensions into account, the change in surface formation energy according to the interfacial adsorption equation[2] is confirmed excellently.

With the obtained dependence of layer-specific segregation on bulk composition, it is shown that segregation cannot be described sufficiently by the single-parameter McLean model. Thus, an analytic layer-specific model of surface segregation is proposed which is capable of reproducing the simulated segregation data over the whole composition range with high accuracy. Using the modeled segregation curves, the change in formation energy can be described in an accurate manner as well.

[1] S. M. Eich, D. Beinke, and G. Schmitz, Comput. Mater. Sci. 104, 185 (2015).
[2] T. Frolov and Y. Mishin, Phys. Rev. B 85, 224106 (2012).

MM 16.8   Tue 12:15   H45

Atomistic simulation of bulk and grain boundaries diffusion in iron — •Sergei Starikov, Matous Mrovec, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-University, Bochum, Germany

In this work, we have studied the grain boundary (GB) diffusion of the point defect and self-diffusion in pure iron. We performed the simulations with different interatomic potentials. The results of classical molecular dynamics were compared with the data calculated with DFT and BOP models. As results we have obtained that GB self-diffusion is controlled by self-interstitial atoms, while the vacancies play major role at bulk diffusion. In addition, exchange mechanism of atomic diffusion takes place for the GB with high energies. Such defectless mechanism of diffusion leads to large self-diffusion coefficient that is in 5-7 orders higher that the bulk one. The comparison with available experimental data was performed.

MM 16.9   Tue 12:30   H45

Modelling of Magnetic Driving Force in Grain Boundary Migration: Using Multi-Phase Field Method — •Liu Huo, Raphael Schiedung, and Ingo Steinbach — Interdisciplinary Centre for Advanced Materials Simulation

We provide a method which combines the dynamical solution of the magnetic moments and multi-phase field method. In our work we solve the motion of magnetic moments using either Time-

Dependent Ginzburg Landau equation or Landau-Lifshitz-Gilbert equation. Meanwhile, by taking advantage of the multi-phase field method, we can solve the magnetic driving force by simply calculate the functional derivative with respect to the phase field for each terms of magnetic free energy so that we are able to solve the magnetic driven grain boundary migration simultaneously. With this method it is possible to simulate some magnetic dependent problems such as the orientation selection in external magnetic field during annealing and the magnetostriction. Our code is implemented in Openphase (www.openphase.de).

MM 16.10   Tue 12:45   H45

Determining mobilities and anisotropic grain boundary energies from MD simulations of shrinking grains — •Adrian A. Schratt and Volker Mohles — ICAMS, Ruhr-Universität Bochum

A new technique to determine average grain boundary (GB) mobilities and energies for arbitrary grain misorientations from molecular dynamics (MD) simulations has been developed. The shrinkage velocity of a cylindrical or spherical grain (2D/3D) allows to calculate the reduced mobility of the GB. From an isotropic model for the capillary driving force we can also derive the average energy of the GB during the shrinkage. The connection between the shrinkage velocity, the GB stiffness and the mobility is exploited to compute the latter. The technique is free of possible artefacts from synthetic driving forces as the GB is only driven by its curvature. In addition, information on the anisotropy of the GB energy can be derived: during shrinkage, the initially cylindrical or spherical shape becomes slightly facetted. This can be expressed as an occurrence frequency of GB plane orientations, which in turn can be used to formulate the GB energy as a function of the plane normal direction. This can be used for instance in mesoscopic models of GB motion.

MM 16.11   Tue 13:00   H45

Simulations of anisotropy effects of interface energies — •Volker Mohles and Adrian A. Schratt — ICAMS, Ruhr-Universität Bochum

Grains and particles of secondary phases control numerous properties of metallic materials. For instance, the interaction between particles and grain boundaries affects recrystallization during heat treatments of manufacturing in a very sensitive manner, which in turn control the material strength and formability. In general, the interface energy of particles and grain boundaries depends on their local orientation in relation to crystallographic planes. This anisotropy strongly affects the equilibrium shapes of particles and grains, hence it can influence the overall properties. In the present contribution, new mesoscopic 2-D and 3-D front tracking simulations of grain boundaries and particle interfaces are presented in which the anisotropy of the interface energy is fully taken into account. It is demonstrated that anisotropic interface energies derived from Molecular Dynamics simulations can be used directly to simulate the resulting particle or grain shapes. The facetting observed in the mesoscopic simulations agrees very well with the corresponding MD simulations. Hence together these simulations provide a multi-scale path toward an improved quantitative understanding of recrystallization kinetics or grain growth, which, for instance, helps improving manufacturing processes of e.g. aluminium sheet. Also, the mesoscopic simulations allow to interpret anisotropic grain boundary energies directly from experimentally observed particle or grain shapes.

MM 17: Nanomaterials

Sessions: Nanomaterials I and II

Time: Tuesday 10:15–13:00   Location: H46

MM 17.1   Tue 10:15   H46

Vacancy-controlled design of MoN/TaN superlattices — Nikola Koutná[1,2], Rainer Hahn[1], Jakub Zálešák[3], Martin Friák[2], Matthias Bartosik[1], Jozef Keckes[3], Mojmír Šob[2], Paul Mayrhofer[1], and •David Holec[3] — [1]Institute of Materials Science and Technology, TU Wien, Vienna, Austria — [2]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [3]Department of Materials Science, Montanuniversität Leoben, Leoben, Austria

Superlattices are effective though experimentally simply-enough accessible microstructural design which allows tuning phase stability and mechanical properties beyond limits of their parent phases. In this contribution we report on our first principles calculations focusing on MoN and TaN, both of which prefer vacancies in their cubic-structured bulk forms. Interestingly, the vacancies strongly segregate to the MoN phase when combined with TaN into superlattices with bi-layer periods in a nm range. This trend based on energetics is further confirmed by evaluating mechanical stability based on elastic constants as well as dynamical stability from lattice vibrations. As a results, we could predict that the most stable configuration for typical conditions during magnetron sputtering, should be MoN_x/TaN system with N vacancies in the MoN phase. This theoretical prediction was experimentally confirmed by X-ray diffraction and an elemental analysis in transmission electron microscope for our reactively-sputtered superlattices.

MM 17.2   Tue 10:30   H46

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

Nanoporous gold (NPG) is an attractive model system for small scale material behavior. The feature size of the chemical stabile, network like structure is tunable from a few to several hundred nanometers. Remarkable are clear distinctions in stiffness and strength, occurring by variations of the solid fraction, ϕ. Yet, due to different processing approaches, the published data are restricted in comparability. A comparative study of the initial composition of precursor alloys, which controls ϕ, and the processing steps is indispensable.
We systematically varied the alloy composition of Au_xAg_{100-x}, with $x = 20, 25, 30, 35$ and we also varied the dealloying procedure with electrochemical corrosion in 1M $HClO_4$ and free corrosion in concentrated HNO_3. Using compression tests with continuous loading and load/unload protocols, we explored the stress-strain behavior, Young's modulus and Poisson's ratio, emphasizing comparability. We confirm significant dependences on the master alloy compositions and show a database of the variation of the mechanical response with ϕ for a given ligament size and push the current approaches to stiffness and strength of nanoscale metal networks forward.

MM 17.3   Tue 10:45   H46

Nanoporous Copper-Nickel - Macroscopic bodies of a strong and deformable nanoporous base metal by dealloying — •Lukas Lührs[1] and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology — [2]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht

In the field of nanostructured materials, nanoporous metals offer significant functionalization potential due to their high surface area to volume ratio. Profiting from high structural definition, potential applications arise as actuators, sensors and structural materials with tunable mechanical properties. Following material characteristics have to be met in these fields: Affordability is an obvious requirement as well as resistance against corrosion, most importantly when potential cycles in electrolyte provide the functionalization. Lastly, deformability is required for avoiding premature failure upon exposure to stress concentrations. So far, macroscopic samples of nanoporous metals with a high surface area and deformability have been limited to precious, and thereby costly, metals such as Au, Pd and Pt.

Here we present nanoporous Copper-Nickel (npCN), a nanoporous base metal that can be made in macroscopic dimensions. Fabricated through dealloying in aqueous media, npCN exhibits a uniform, bicontinous network structure with feature sizes that can be controlled from 13 to 40 nm by thermal annealing. Compression tests find ductile deformation behavior accompanied with a high strength compared to other nanoporous base metals as well as macroporous Cu- and Ni-

foams.

MM 17.4 Tue 11:00 H46

Electrosorption in Polypyrrole-Silicon Hybrid Nanopores: Insights from Cyclic Voltammetry and Dilatometry — •Manuel Brinker[1], Guido Dittrich[1], Pirmin Lakner[2], Thomas Keller[2], and Patrick Huber[1] — [1]Technische Universität Hamburg — [2]Deutsches Elektronen-Synchrotron DESY

Porous silicon provides a scaffold structure to study confinement effects of soft matter, since the pore diameter, pore length and pore shape can be tuned in a wide range. We investigate the electrosorption of electrolyte anions and the electrochemical behaviour of nanoporous silicon in acidic electrolytes. The silicon-electrolyte interface acts as a capacitor which allows the accumulation of electrolyte anions in a chemical double layer by an applied voltage. The sorption characteristics can be measured by cyclic voltammetry. The surface stresses that emerge in a monolithic porous silicon membrane by electrosorption lead to a macroscopic strain which can be measured in-situ with a dilatometer. Furthermore, we investigate the properties of a functional filling of the electrically conductive polymer polypyrrole (PPy) into nanoporous silicon. We successfully demonstrate the filling of PPy into pores of substantial depth of up to 100 μm. In particular, PPy allows for sensoric and actoric applications for the hybrid system. PPy swells when it is exposed to a voltage in an electrolyte, since ions from the electrolyte are intercalated into the polymer structure and expelled subsequently. The confinement effect of the pores on the swelling can be studied with dilatometry measurements as well and is compared to the nanoporous silicon itself.

MM 17.5 Tue 11:15 H46

Sorbitol capping of gadolinium oxide nanoparticles for contrast enhancement in magnetic resonance imaging — •Natalia Abrikosova[1,2], Caroline Brommesson[2], Peter Eriksson[2], Zhangjun Hu[2], and Kajsa Uvdal[2] — [1]Materials Modeling and Development Laboratory, National University of Science and Technology ”MISIS”, 119049 Moscow, Russia — [2]Department of Physics, Chemistry, and Biology (IFM), Linköping University, SE-58183 Linköping, Sweden,

Diagnostic with magnetic resonance imaging (MRI) is the method of choice to detect diseases accompanied by an inflammation within the body. MRI contrast agents based on magnetic nanoparticles represent an efficient tool to improve image quality by enhancing the contrast between normal and diseased tissue, thereby increasing the utility of MRI. In this work, we report an investigation of the effect of sorbitol on the performance of Gd-oxide nanoparticles (GdNPs) as MRI contrast agents. Two sets of experiments were performed, where GdNPs were either capped to or immersed in sorbitol. The longitudinal relaxation rates for hematopoietic cell samples, were measured. The results show that the presence of sorbitol as capping layer on GdNPs clearly improves the nanoparticle performance. Moreover, measurements on human neutrophil granulocytes and the production of reactive oxygen species (ROS), evidently demonstrate improved biocompatibility of the GdNPs capped with sorbitol. We hereby conclude that the strategy to cap nanoparticles with sorbitol is a promising pathway in search for the next generation of MRI contrast agents.

MM 17.6 Tue 11:30 H46

Atom probe analysis of nanoparticles: development of new sample preparation methods — •Jan Paul Josten and Peter Felfer — Department Materials Science and Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg, Institute I, Martensstraße 5, 91058 Erlangen, Germany

Atom probe tomography (APT) of nanoparticles (NPs) has shown great potential with its atomic resolution for chemical and structural characterization. [1] Two novel methods are used to produce NP APT samples. First, the so called 'stamping transfer' (ST) [2] is used that was originally developed to produce free standing micro- and NPs on top of tip substrates for electron tomography by an in-situ SEM procedure. Second, based on an approach where single NPs have been attached to field emitters inside the analysis chamber [3] we developed a field ion microscope set-up (ES-FIM) where NPs can be introduced into ultra-high vacuum (UHV) as an electrospray aerosol through a transfer system. In order to understand the NP-APT sample set-up, field evaporation simulation using models developed at Group des Materiaux (GPM) by Vurpillot et al. [4,5] are used and results presented along with first experimental results and a comparison of the two methods to already existing methods.

[1] Tedsree, K. et al.; Nat. Nanotechnol. **2011** 6, 302-307
[2] Przybilla, T. et al.; Small Methods **2018** 2, 1700276
[3] Castro, T. et al.; J. Vac. Sci. Technol. **1989** 7, 2845-2849
[4] Vurpillot F., et al.; Ultramicroscopy **2000** 84, 213-224
[5] Rolland N., et al.; Microsc. Microanal. **2015** 6, 1649-1656

15 min. break

MM 17.7 Tue 12:00 H46

Spin, angle and time-resolved photoemission studies of WTe$_2$ and WSe$_2$ — •Jakub Schusser[1,2], Jan Minar[2], Maria Christine Richter[1], Mauro Fanculli[1], Olivier Heckmann[1], Laurent Nicolai[2], Waly Ndiaye[1], Zakariae El Youbi[1], Thierry Ruchon[3], David Bresteau[3], and Karol Hricovini[1] — [1]LPMS, University of Cergy-Pontoise, Neuville-sur-Oise, France — [2]University of West-Bohemia, New Technologies Centre, Pilsen, Czech Republic — [3]ATTOLab, CEA, Saint-Aubin, France

Molybdenum dichalcogenides are probably the most studied single layer TMDCs by virtue of being appealing for sundry possible applications suchlike transistors, diodes, solar cells or more fundamental studies of spin or valley pseudospin and their interactions. Tungsten-based counterparts are on the other hand evincing much stronger spin-orbit coupling due to which all the spin-related effects are more stable at room temperature and thus more feasible for application. We have conducted several experiments following the evolution of the spin texture near the X, Y, K and M points of the Brillouin zone (WTe$_2$ and WSe$_2$ respectively) which is substantial for understanding the fundamental properties of the structure-property relation of the system. Ab-initio set of photoemission calculations was also performed using SPR-KKR package. Furthermore, TR-SARPES studies will be carried out by the group on such materials to determine the ultrafast dynamics of the carrier density and to disentangle the subsequent relaxation processes using pump-probe experiments.

MM 17.8 Tue 12:15 H46

Towards plasmonic tunnel gaps for nanoscale photoemission currents by on-chip laser ablation — Philipp Zimmermann[1,2], •Alexander Hötger[1], Noelia Fernandez[1], Reinhard Kienberger[3,4], and Alexander Holleitner[1,2] — [1]Walter Schottky Institute and Physics Department, Technical University of Munich, Am Coulombwall 4a, 85748 Garching, Germany — [2]Nanoinitiative Munich (NIM), Schellingstr. 4, 80799 München, Germany — [3]Physics Department E11, Technical University of Munich, James-Franck-Str. 1, 85748 Garching, Germany — [4]Max-Planck-Institute für Quantenoptik, Hans Kopfermann-Straße 1, 85748 Garching, Germany

We demonstrate that prestructured metal nanogaps can be shaped on-chip to below 10 nm by femtosecond laser ablation. We explore the plasmonic properties and the non-linear photocurrent characteristics of the formed tunnel junctions. The photocurrent can be tuned from multi-photon absorption towards the strong-field tunneling regime in the nanogaps. We demonstrate that a unipolar ballistic electron current is achieved by designing the plasmonic junctions to be asymmetric, which allows ultrafast electronics on the nanometer scale.

MM 17.9 Tue 12:30 H46

The Effect of Molecular Orientation on the Plasmon Resonance of Metal Nanostructures — •Thomas Purcell[1], Shira Yochelis[2], Yossi Paltiel[2], and Tamar Seideman[1] — [1]Chemistry Department, Northwestern University, Evanston, IL, USA — [2]Applied Physics Department and the Center for Nanoscience and Nanotechnology, Hebrew University of Jerusalem, Jerusalem, Israel

Plasmon-based nanophotonics is becoming increasingly popular, in part because of its ability to improve the efficiency of optical devices by enhancing electromagnetic fields near plasmonic hot-spots~[1]. To fully describe the plasmonic enhancement in these devices, contributions from both the sensitizers and the nanostructures need to be accounted for. Modeling the coupling between those two contributions, including the often decisive alignment between the sensitizers' and plasmon's dipole moments, remains an open challenge. By modifying the finite-difference time-domain method we develop a continuous model for a layer of molecular dipoles with an arbitrary orientation relative to a nanoparticle's surface, and study the coupled system's optical~[2] and chiroptical~[3] response. We demonstrate how the molecules alter the plasmon resonance of nanostructures and change the coupling between the plasmon and a colloidal quantum dot mono-

layer. Finally we include chiroptical effects to get a better understanding how the molecular dipole orientation affects chiral imprinting inside nanoparticles.

[1] T. Purcell, et al., J. Phys. Chem., 120, 21837 (2016)
[2] T. Purcell, et al., J. Phys. Chem., 122, 16901 (2018)
[3] T. Purcell and T. Seideman, ACS Photonics, Accepted

MM 17.10   Tue 12:45   H46

static friction vs young's modulus: the essential factors in reusable anodic aluminum oxide (AAO) template as a master mold — •Huanming Zhang, Min Zhou, Yang Xu, Rui Xu, Zhiqiang Zeng, and Yong Lei — Institute für Physics & IMN Macro-Nano (ZIK), Technische Universität Ilmenau, 98693 Ilmenau

To construct ordered nanostructure over a large area, Anodic Aluminum Oxide (AAO) template-directed fabrication is a promising technology. Herein, we propose a facial method to fabricate highly ordered metal film with AAO template as a master mold. After metal deposition in the AAO pores, the ordered metal films can be easily obtained by mechanical stripping from AAO template. To obtain a complete metal film, control experiments were conducted, and the aspect of the pore in AAO template and the Young's modulus of the metal deposited in the AAO pores was supposed to be the essential factors. The aspect-dependent static friction interacts with Young's modulus of the metal deposited in the AAO pores closely.

MM 18: Interfaces

Time: Tuesday 14:15–15:30   Location: H45

MM 18.1   Tue 14:15   H45

Influence of Ta and Zr segregation on the atomic structure of [111] tilt grain boundaries in Copper — •Thorsten Meiners, Christian H. Liebscher, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf

Recently, nanocrystalline Copper (Cu) has been investigated intensively, because of its excellent properties such as high strength and hardness. However, at elevated temperatures rapid grain growth causes a destabilization of the microstructure. Therefore, alloying Cu with immiscible elements such as Zr and Ta has shown to greatly stabilize the microstructure induced by strong grain boundary (GB) segregation and precipitation. In our study we investigate the atomic structure of these GB segregation and precipitation phenomena at [111] tilt GBs in Cu by aberration-corrected (scanning) transmission electron microscopy in order to identify the atomistic mechanisms of the microstructure stabilization. We found spherical Ta_{x}O nano particles at the GBs, which locally distort the GB plane and can thus lead to Zener pinning. Zr is found to form a kind of glass-phase, which is inhomogenously distributed at the GBs. Especially GB steps are strongly decorated with nanometer sized Zr-rich inclusions. In addition we observe Zr-induced structural transitions compared to clean GBs, indicating that these local chemical states alter the GB properties.

MM 18.2   Tue 14:30   H45

Partitioning of segregating impurities during grain boundary decohesion — Xiang Huang[1,2], Alexander Hartmaier[1], and •Rebecca Janisch[1] — [1]ICAMS, Ruhr-Universität Bochum, Germany — [2]Department of Chemistry, Technical University Munich, Germany

The embrittling effect of hydrogen atoms at grain boundaries is widely studied by means of density functional theory calculations. A first indicator on the effect of H on the interface cohesion is the change in the work of separation due to the impurity. The work of separation is simply the difference between the energy of the two free surfaces after a brittle cleavage of the interface, and the grain boundary energy. However, in the case of a grain boundary with segregated impurities and/or alloying atoms, several possibilities exist of how to distribute the segregants on the two surfaces. In this work we demonstrate the striking effect of different partition patterns and additional surface diffusion on the final effect of C and H atoms on the cohesive behavior of a bcc Fe Σ3(112)[110] symmetrical grain boundary. The change in the work of separation is further analyzed by decomposition into chemical and mechanical contribution according to the thermodynamic theory of Rice and Wang.

MM 18.3   Tue 14:45   H45

Amorphous interlayers in semiconductor metallization — •Dennis König, Efi Hadjixenophontos, Guido Schmitz, and Kevin Treder — Institute of Materials Sience, Chair of Material Physics, University of Stuttgart, Heisenbergstraße 3, 70569, Germany

Deposition of thin metallic films on monocrystalline silicon substrates has been extensively used in the past. An amorphous interlayer of few nm, between the silicon and the metallic coating is reported in such systems. During this work detailed investigation on this interlayer is done. Different parameters are studied such as: The cleaning time of the substrates, the power during deposition and the metallic element (Al, Au and Ag) in contact with the substrate. Samples are prepared by Ion beam sputtering with controlled thicknesses and are characterized by HRTEM after FIB cross sections. Further elemental analysis is done by EDX during microscopy. A clear dependency of the thickness of interlayer is observed on the cleaning time and power during deposition. Attempts to identify the composition of the amorphous interlayer are performed by Atom Probe Tomography.

MM 18.4   Tue 15:00   H45

A quantum-mechanical study of connections between tensorial elastic properties and chemical bonds in Σ5(210) grain boundaries in Ni$_3$Si compound — •Martin Friák[1], Martin Zelený[2,3], Monika Všianská[4,1,5], David Holec[6], and Mojmír Šob[5,1,4] — [1]Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic — [2]Institute of Materials Science and Engineering, NETME Centre, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [3]Faculty of Mathematics and Physics, Charles University in Prague, Prague, Czech Republic — [4]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [5]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic — [6]Department of Materials Science, Montanuniversität Leoben, Leoben, Austria

Using *ab initio* methods we calculate and analyze (tensorial) anisotropic elastic properties of interface states associated with Σ5(210) grain boundaries (GBs) in cubic L1$_2$-structure Ni$_3$Si. In particular, we show that GB variant containing both Ni and Si atoms at the interface is unstable with respect to a shear deformation (one of the elastic constants, C_{55}, is negative). Our elastic-constant analysis allowed us to identify a shear-deformation mode reducing the energy and eventually to obtain mechanically stable ground-state. We further discuss an atomistic origin of this instability in terms of the crystal orbital Hamilton population (COHP) and phonon dispersion calculations. For details see Friák *et al.* Materials 11 (2018) 2263.

MM 18.5   Tue 15:15   H45

Size independent description of the strain effects on the segregation of carbon and hydrogen in iron — •Abril Azócar Guzmán, Alexander Hartmaier, and Rebecca Janisch — ICAMS, Ruhr-Universität, Bochum, Germany

Structural materials such as steels are frequently processed under stress and strain conditions; in such systems, C and H have been shown to strongly affect the mechanical properties of Fe. Therefore, it is of interest to understand the coupling between segregation phenomena and mechanical response. In this work, we study the cohesion behaviour of a Σ5(310)[001] symmetrical tilt grain boundary (STGB) in body centred cubic (bcc) Fe with C as an interstitial alloying element and H as an impurity. Using first-principles calculations, the solution and segregation energies are obtained for varying mechanical load and GB coverage of the segregating atoms, either for fixed concentration or fixed chemical potential. Thus, the maximum concentration of C and H is calculated. We discuss that the concept of strain, or displacement, in *ab initio* tensile tests that include structural relaxations is ill-defined due to the release of elastic energy, which causes the calculated total energies to depend on the system size. The proposed procedure is to obtain the solution energies as a function of the stress instead of the displacement (or strain), assuming that the stress distributes equally among crystallographic planes in the supercell.

MM 19: Miscellaneous: Biomaterials, Magnetic Shape Memory Alloys, Sensors and Actuators (joint session MM/MA)

Time: Tuesday 14:15–15:45   Location: H46

MM 19.1 Tue 14:15 H46
Magnetic and chemical microstructures of Mn-based Heusler compounds studied by small-angle neutron scattering — •Ulrike Zweck, Michael Leitner, Pascal Neibecker, and Winfried Petry — Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching

Ni_2MnZ based Heusler compounds have attracted a considerable amount of attention due to their various appealing properties such as the ferromagnetic shape-memory effect or the magnetocaloric effect. Since the magnetic properties are very sensitive to the degree of structural order in these systems [1], understanding the correlation of these two ordering parameters is crucial.

The magnetic moments are mainly carried by the Mn atoms, which interact ferromagnetically in the $L2_1$-ordered state. However, it has been found that at structural anti-phase domain boundaries the magnetization tends to reverse, leading to atomically sharp ferromagnetic domain walls [2]. To study this interplay of magnetic and structural order as well as the mechanism of coupling of ferromagnetic domains across APD boundaries, we have investigated Ni_2MnAl and $Ni_2MnAl_{0.5}Ga_{0.5}$ powder samples in distinct ordering states via temperature-dependent small-angle neutron scattering (SANS), giving access to the magnetization microstructure. Further, we reproduce the correlation between structural and magnetic order by Monte Carlo simulations.

[1] P. Neibecker *et al.*, Appl. Phys. Lett. **105**, 261904 (2014).
[2] H. Ishikawa *et al.*, Acta Mater. **56**, 4789 (2008).

MM 19.2 Tue 14:30 H46
Atomic disorder in magnetocaloric materials: A roadmap for achieving better performance — •Biswanath Dutta[1,2], Bruno Weise[3], Niclas Teichert[4], Andreas Hütten[4], Anja Waske[3], Fritz Körmann[1,2], Tilmann Hickel[2], and Jörg Neugebauer[2] — [1]Materials Science and Engineering, Delft University of Technology, Delft, Netherlands — [2]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [3]Institute for Complex Materials, IFW Dresden, Dresden, Germany — [4]Department of Physics, Bielefeld University, Bielefeld, Germany

Understanding and improving magnetic properties of magnetocaloric materials is of great importance for their practical applications. In the quest to enhance these properties, different design strategies have been employed in recent years. Using ab initio calculations, we study the impact of atomic disorder on the martensitic transformation and the magnetic properties in Ni-Mn-based magnetic shape memory alloys (B. Weise et al., Sci. Rep. 8:9147 (2018)). The calculations reveal a remarkable impact of atomic configuration on the structural and magnetic properties of the cubic austenite phase. We also find a delicate interplay of magnetic and chemical orders and the tetragonal distortion during the martensitic transformation, explaining the giant inverse magnetocaloric effect in these alloys. Based on these findings, we qualitatively explain the experimentally observed changes in the magnetocaloric properties after different annealing times. Our investigations thus provide a promising route, i.e., managing disorder with optimal annealing to achieve better magnetocaloric properties.

MM 19.3 Tue 14:45 H46
Stretchable Multidimensional Magnetic-Triboelectric Electronic Skin — •Tianxiao Xiao, Gilbert Santiago Cañón Bermúdez, Jürgen Fassbender, and Denys Makarov — Helmholtz-Zentrum Dresden-Rossendorf e.V., Dresden, Germany

Owing to their unique mechanical properties and abilities of touchless interaction with physical and virtual objects [1-3], magnetic field sensors became an integral part of the electronic skins (e-skins) concept [4,5]. In this work, we report a stretchable magnetic-triboelectric electronic skin (MTES) by the combination of giant magnetoresistive (GMR) sensors and triboelectric nanogenerators (TENG). Here, Co/Cu multilayers and polydimethylsiloxane (PDMS) layer not only form a flexible GMR sensor system but also serve as the electrode and dielectric layer of a single-electrode TENG. This work demonstrates the first sensor system based on both magnetic and triboelectric effects. [1] Makarov, D., et al., Appl. Phys. Rev. 3, 011101 (2016). [2] Cañón Bermúdez, G. S., et al., Nature Electronics 1, 589 (2018). [3]

Cañón Bermúdez, G. S., et al., Science Advances 4, eaao2623 (2018). [4] Chortos, A., et al., Nature Materials 15, 937 (2016). [5] Amjadi, M., et al., Adv. Funct. Mater. 26, 1678 (2016).

MM 19.4 Tue 15:00 H46
Hybrid Materials Made from Nanoporous Metals and Electrically Conductive Polymers as Electro-Chemo-Mechanical Actuators — •Benedikt Roschning[1] and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — [2]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

Nanoporous metals can be used as functional materials like sensors or actuators, due to their high intrinsic, externally accessible surface. The mechanism is based on surface stress variations as a consequence of an applied electrical potential. This stress variation acts on the underlying bulk atoms, resulting in actuation, scaling with the feature size. The environmental stability and structural coarsening due to surface diffusion restricts the materials choice to noble metals like gold or platinum and are still an issue in terms of long-term stability.

Another class of electro-chemo-mechanical actuators are conductive polymers. Their actuation is caused by the incorporation of co-ions between the polymer chains for charge balancing. Within thin films, fast ion exchange is possible, but the stiffness of the underlying substrate limits the effect of actuation.

A combination of both approaches, the coating of the intrinsic surface area of nanoporous metals with electrically conductive polymers, leads to superior electrochemical and actuatoric properties. Within this contribution, we address manufacturing approaches, the electrochemical properties as well as the underlying mechanisms for actuation.

MM 19.5 Tue 15:15 H46
Platform for quantitative analysis of biochemical processes in droplets using nano-sensors. — •Dmitry Belyaev[1], Larysa Baraban[1,2], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science TU Dresden, MBZ, Budapester Str. 27, 01069, Dresden, Germany — [2]Technische Universität Dresden Center for Advancing Electronics Dresden, 01062, Dresden, Germany

Real time monitoring of bio-chemical reactions and processes, e.g. related to the cancer development is highly relevant. This, can be done by implementing miniaturized lab-on-a-chip detecting systems, incorporating microfluidics and Si nanowire field effect transistor (SiNW FET) chip allowing droplet analysis[1]. Here, the chemical reaction of β-galactosidase and ortho-nitrophenol-galactose (ONPG) was detected in a label free format, and the kinetics was analyzed using SiNW EFT. SiNW FET is ion sensitive device and it is able to detect presence of charged molecules or ions in the liquid environment. The reaction was analyzed in a numerous emulsion droplets generated in a microfluidic flow-cell, by means of honeycomb shaped NW FET chip. The flow cell was produced via combination of laser, UV and soft lithography techniques and consists of the droplets generation module and the channel structure with width of about $300\mu m$, and is successfully integrated on silicon chip. We attribute the shift of the Isd current to the change on ionic composition of the media. Comparative data proved successful detection of the reaction.

1)J. Schütt et al., Nano Lett. 2016, 16, 8, 4991-5000

MM 19.6 Tue 15:30 H46
Diamond-based materials interacting with DNA units — Miftahussurur Hamidi Putra[1], Di Liu[1], Chandra Shekar Sarap[1], Pouya Partovi-Azar[2], and •Maria Fyta[1] — [1]Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany — [2]Institute of Chemistry, Martin Luther University Halle-Wittenberg, 06120 Halle (Saale), Germany

Using quantum-mechanical calculations implementing density functional theory, we model the interaction of DNA units with diamond-based structures. For the former, we consider the DNA canonical nucleobases and nucleotides, as well as their modified counterparts. For the material part, we focus on terminated surfaces and nanodiamonds. The latter involve defective spherical diamond particles, as well as diamond-cages, known as diamondoids. We model the interactions of

these material structures to the DNA units taking into account the surface termination, bonding arrangement and DNA type. Through our computations, we assess the binding strength, electronic properties, as well as optical spectra and charge dynamics of these diamond/DNA

hybrid complexes. In the end, we discuss the relevance of such hybrid materials in realizing novel biosensors for the detection of DNA sequences and their mutations.

MM 20: Poster session II

Time: Tuesday 18:30–20:00   Location: Poster C

MM 20.1   Tue 18:30   Poster C

Tuning mechanical stress by nano-structure — •Philipp Klose[1,2], Magnus Hamm[1], Stefan Wagner[2], and Astrid Pundt[1,2] — [1]Institut für Materialphysik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Institut für angewandte Materialien IAM-WK, Karlsruher Institut für Technologie, Engelbert-Arnold-Straße 4, 76131 Karlsruhe

When materials are adhered to rigid substrates, the sorption of light elements can lead to high mechanical in-plane stress.[1,2] Linear elastic theory predicts stresses in the range of -10 GPa, for 1 Hydrogen atom in Niobium.[1,2] These stresses can lead to changes in the material's properties. For low element concentrations, the mechanical stress increases linearly by the element content. However, reduction in the stress increase appear at and above the yield stress.[3] Final stress of about -3 GPa are commonly measured. The final stress can be tuned by decreasing the film thickness. For Nb films below 6 nm, linear and reversible stress increase is maintained to 1 H/Nb and mechanical stress of about -10 GPa is actually measured.[4] The range of linear elasticity can be increased to about 80 nm film thickness, by varying the lateral domain size.[5,6] This will be done by a coherently matched second phase. This work is financially supported by the DFG via project PU131/12-1. [1] U. Laudahn et al., JALCOM (1999), [2] S. Wagner et al., Appl. Phys. Lett. 92 (2008), [3] A. Pundt et al., Phys. Rev. B 61.15 (2000), [4] Hamm, M., et al. APL 106 (2015), [5] P. Klose et al. IJHE (2017),[6] P. Klose et al., submitted.

MM 20.2   Tue 18:30   Poster C

Residual Silver in Nanoporous Gold prepared by Alloy Corrosion — Mareike Haensch[1], Matthias Graf[2], •Weijia Wang[3], Alexei Nefedov[3], Christof Woell[3], and Gunther Wittstock[1] — [1]Karl von Ossietzky University of Oldenburg, Institute of Chemistry, Oldenburg, Germany — [2]Hamburg University of Technology, Institute of Optical and Electronic Materials, Hamburg, Germany — [3]Karlsruhe Institute of Technology, Institute of Functional Interfaces,Eggenstein-Leopoldshafen, Germany

Nanoporous gold (NPG), a nanoporous bulk material, finds applications in electrocatalysis, sensing and energy storage/conversion due to its large surface-to-volume ratio, good electrical conductivity, high catalytic activity and chemical/structural flexibility. Samples with homogeneous structures up to several mm in size can be obtained by dealloying a silver-gold alloy in concentrated nitric acid or by applying a potential program. However, the dealloying process is never complete. The dealloyed NPG contains a residual fraction of silver, which can affect its catalytic properties. A recent TEM study shows that the residual silver is present in silver-rich regions which are remnants of the parent alloy. The depth distribution of these regions is still under debate.XPS with variation of the excitation photon energy was used to identify depth-dependent distribution of residual silver. NPG samples which underwent different treatments were investigated. For all samples the silver enrichment was found at the surface, which is in agreement with previous studies.

MM 20.3   Tue 18:30   Poster C

synthesis and optical characterization of plasmonic nanoparticles — •Ricardo Baez[1,2], Paulraj Manidurai[2], Shirly Espinoza[3], and Charusheela Ramanan[1] — [1]Max Planck Institute for Polymer Research; Department -Molecular Electronics, Ultrafast Spectroscopy for Optoelectronics. Ackermannweg 10, 55128 Mainz, Germany. — [2]Department of Physics, Faculty of Physical and Mathematical sciences, PO box-160-C, University of Concepcion, Concepcion, Chile. — [3]ELI Beamlines, Institute of Physics, Czech Academy of Science, Na Slovance 2, 18221 Prague, Czechia.

Gold nanoparticles have promising potential for photonic applications due to high chemical stability and strong optical cross-sections [1,2]. These colloidal nanoparticles present a stable localized plasmon reso-

nance (LPR), which leads to an enhancement of scattering processes of up to 1015 orders of magnitude [4]. In the present work we carried out a synthesis of gold nanoparticles (AuNPs) via a microwave-assisted technique using natural Vitamin C as the reducing agent [5]. Only water, Vitamin C and the gold salt precursor are necessary to generate the AuNPs under the influence of microwaves [6]. Previous results have shown the possibility of controlling the shape/size of colloids using variations in radiation time. TEM micrographs reveal stable triangular, spherical, and pentagonal morphologies, with varying distribution and size [7].The optical properties have been studied by using absorption and fluorescence spectroscopy [8,9]. Theoretical calculations have been by using boundary element method (BEM) [10].

MM 20.4   Tue 18:30   Poster C

Improving the stability of Silver Nanowires for electrodes via surface modification — •Violetta Kalancha[1], Ievgen Levchuk[1], Nadine Schrenker[2], Erdmann Spiecker[2], Christoph J. Brabec[1], and Karen Forberich[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Materials for Electronics and Energy Technology (i-MEET), Martensstrasse 7, 91058 Erlangen, Germany — [2]Institute of Micro- and Nanostructure Research and Center for Nanoanalysis and Electron Microscopy (CENEM), Cauerstr. 6a, 91058 Erlangen, Germany

The future electronic devices will be soft, flexible and even stretchable to be more human friendly in the form of wearable computers and gadgets. Transparent conductors are currently made from a sputtered film of indium tin oxide (ITO) due to its high transmittance (95In this context, we are planning to develop a highly reproducible method of homogeneous silver nanowire synthesis with further surface functionalization by ligand exchange of organic ligands to inorganic ligands. We believe that this ligand exchange of original NWs surface ligands (PVP) can provide better interwire charge transport as well as material stability. Next, this modified Ag NWs will be investigated both in film and solution. The recent progress consists of a modified polyol synthesis resulting in Ag NWs with average diameters of 30 nm and length up to 50 μm. High-performance transparent electrodes require thin diameter and high aspect ratio as two key structural traits that determine their film performance. References: 1.*Ye al., Adv. Mater. 2014, 26, 6670. 2.*Li et al., Nano Lett. 2015, 15, 6722*6726

MM 20.5   Tue 18:30   Poster C

Tailoring microstructure of Ni-Mn-Ga single crystals through thermo-magneto-mechanical treatment — •Jonas Heider[1,2], Emmanouel Pagounis[2], Robert Chulist[3], Markus Laufenberg[2], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]ETO MAGNETIC GmbH, Hardtring 8, 78333 Stockach, Germany — [3]Institute of Metallurgy and Materials Science, Polish Academy of Sciences, 30-059 Krakow, Poland

Magnetic shape memory alloys (MSMA) are a promising type of smart material for application in actuators, sensors and energy harvesting devices due to their giant and fast strain induced by a moderate magnetic field or external stress. This strain is based on the motion of twin boundaries of adjoining martensitic twin variants with different orientations. A wide range of materials with varying modulations have been discovered exhibiting magnetic-field-induced strain (MFIS). Among those the Ni-Mn-Ga composition is the most promising MSMA with up to 7.1% MFIS in the five-layered (10M) modulated martensitic phase.

In our work we address the complex microstructure of adjoining twins in Ni-Mn-Ga single crystals in order to understand how different types of twin boundaries can be prepared, preserved and utilized for applications. Crystallographic analysis considering a monoclinic unit cell is performed to identify fine laminates between the macro-twinning planes denoted a/b-laminates. The evolution of the structure and magnetic properties is investigated depending on the thermo-magneto-mechanical treatment of single crystalline samples.

MM 20.6 Tue 18:30 Poster C

photothermal study of RGO-Ag nanowire composite in solid state — •Nishaina Sahadev and Aji Anappara — dept. of physics, nit calicut, nit campus p.o, calicut, india

Reduced Graphene Oxide (RGO) have been shown to exhibit excellent light-to-heat transduction owing to its broad-band absorptance (IR-to-UV range of frequencies) and negligible photoluminescence. Similarly silver nanowires also exhibit good photothermal activity. Here, we report a comparative study of the photothermal activity of RGO and its composites with Ag nanowires in solid state. While Ag nanowires has its characteristic plasmon absorption peaks at ~377 and 351 nm, RGO exhibits an absorption peak maxima at ~ 272 nm in the UV range corresponding to the M-point in its electronic band structure. A photo-DSC setup with a UV-visible light source (250-450 nm) was used for carrying out isothermal photocalorimetric measurements on the samples at ~ 25 oC. Upon irradiation, the samples RGO, S1 and S2 (S1 and S2 are composites of RGO and Ag nanowires; with different mass percentages of Ag nanowire) in powder form were found to generate considerable amount of heat. An interesting observation was that the mass-normalized heat output of the composites (S1 and S2) upon light irradiation was higher as compared to RGO possibly resulting from the better light absorption in the composites as compared to RGO alone.

MM 20.7 Tue 18:30 Poster C

determination of the miscibility gap of Pt-Pd using Atom Probe Tomography — •Yoonhee Lee and Guido Schmitz — Heisenberstr. 3, 70569 Stuttgart

Understanding the thermodynamics of alloy system is fundamental and a prerequisite to interpret the properties of the materials. So, no surprise that of most binary metallic system the phase diagrams were already well evaluated. Nevertheless, in some cases required data are missing, which holds especially for miscibility gaps at low temperature. A miscibility gap is suggested for Pt-Pd, an important alloy system essential for catalysis. Even though there were many efforts to prove the miscibility gap since Raub [1] have first claimed it with a critical temperature of approximately 770°C, still the gap remains as a dashed unclear line in the published phase diagrams [2].

In this work, we try to overcome the lack of information by applying Atom Probe Tomography (APT) to thin film structures needing only short diffusion length to establish equilibrium. APT is a cutting-edge technology, which can achieve an outstanding three-dimensional spatial resolution. Thus, it enables the study of atomic diffusion on a (sub-)nanometer length scale. Pt and Pd multilayers are deposited via ion beam sputtering and annealed at different temperatures to approach equilibrium. Then, needle-shaped samples are prepared by FIB lift-out and measured in APT. The experimentally determined miscibility gap is presented in comparison to literature data.

[1] *E. Raub, Journal of the Less-Common Meterials, vol. 1, pp. 3-18, 1959. [2] *T. Massalski, Binary Alloy Phase Diagrams, 1990.

MM 20.8 Tue 18:30 Poster C

The Impact of an Effective Triple-line Energy on Solder Reflow and Difficulties in its Quantification — •Samuel Griffiths and Guido Schmitz — Institute for Materials Science, Stuttgart University, Germany

Micro-solder technologies are ubiquitous in modern electronics industries. Although these industries have driven vast practical advancements in solder technologies, little is understood about the impact of miniaturization on the reflow behaviour of solder on metal conductive tracks.

This work investigates the reflow behavior of Sn-based micro-solder on micro-structured Cu and Ni capillary tracks for various track widths. The results are compared both with the ideal wetting model of surface and interface energy equilibrium and a modified model containing a term for an effective triple-line energy which causes the steady state contact angles to deviate from the ideal case. Difficulties surrounding sample production, measurement and analysis are discussed. The difference between general surface roughness and substrate defect sites is discussed in relation to the quantification of an effective triple-line energy. The presence of an effective triple-line energy is confirmed through comparisons between surface energy optimisation modelling and experimental results.

Future work will entail further minimisation of sample dimensions towards a strip width of 1 micrometer and the process to achieve this as well as the inherent difficulties will be discussed.

MM 20.9 Tue 18:30 Poster C

Formation and electronic structure of tetracarbonates under extreme conditions — •Christian Albers[1], Georg Spiekermann[2], Robin Sakrowski[1], Christian Sternemann[1], Max Wilke[2], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, TU Dortmund — [2]Institut für Erd- und Umweltwissenschaften, Universität Potsdam

Iron-bearing carbonates are candidates for carbon storage in the deep Earth, therefore their physical properties and chemistry at high pressure and high temperature are in focus of recent research [1].

We present a setup to establish the conditions in the lower mantle (100 GPa, 3000 K). The required pressure is accomplished by diamond anvil cells [2], in which the sample is heated double-sided by a Nd:YAG-Laser. Via combined X-ray emission and X-ray Raman spectroscopy [3] the electronic structure of the synthesized compounds at high pressure and temperature can be analyzed. Furthermore, optical Raman scattering provides information about the geometric structure. The case of siderite and magnesiosiderite will be discussed.

[1] V. Cerantola et al., Nat. Comm. 8, 15960 (2017)
[2] S. Petigirard et al., J. Synchrotron Rad. 24, 276-282 (2017).
[3] C. Weis et al., Scientific Reports 7, 16526 (2017)

MM 20.10 Tue 18:30 Poster C

Liquid-Infused Nanoporous Solids as Photonic Metamaterials — Kathrin Sentker[1], Mark Busch[1], Andriy V. Kityk[2], and •Patrick Huber[1] — [1]Institute of Materials Physics, Hamburg University of Technology (Germany) — [2]Department of Electrical Engineering, Czestochowa University of Technology (Poland)

Metamaterials derive their functional properties not from the properties of the base materials, but from their newly designed, often multiscale structures, in terms of precise shape, geometry, size, orientation, and elastic properties. Such hybrid material systems can be designed by infusing liquids in porous solids. In particular nanoporous media offer the possibility to establish structures significantly smaller than visible-light wavelengths and thus to act as photonic metamaterials, where the optical properties can be fine-tuned by the filling of the pore space. Here we present Laser-optical, x-ray and neutron diffraction experiments on monolithic nanoporous silicon, silica and alumina filled with simple (n-alkanes, water) and complex liquids (polymers, liquid crystals). These experiments allow us to gain detailed insights on the liquid distribution in the nanoporous media and the phase behaviour of the confined fluids with regard to the unconfined state. By the same token the resulting soft-hard hybrid materials exhibit novel properties typical of photonics metamaterials, encompassing optical birefringence step-wise changing with temperature, switchable optical transmission and fast electro-optical activity.

MM 20.11 Tue 18:30 Poster C

***In situ* TEM in Liquids Using a Si$_3$Ni$_4$ – Graphene Hybrid Cell Design** — •Birk Fritsch[1], Andreas Hutzler[1], Michael P. M. Jank[2], Robert Branscheid[3], Erdmann Spiecker[3], and Martin März[1,2] — [1]Electron Devices (LEB), Department of Electrical, Electronic and Communication Engineering, Friedrich-Alexander University Erlangen-Nürnberg (FAU), Cauerstraße 6, 91058 Erlangen, Germany — [2]Fraunhofer Institute for Integrated Systems and Device Technology IISB, Schottkystraße 10, 91058 Erlangen, Germany — [3]Institute of Micro- and Nanostructure Research (IMN) and Center for Nanoanalysis and Electron Microscopy (CENEM), Department of Materials Science and Engineering, Friedrich-Alexander University Erlangen-Nürnberg (FAU), Cauerstraße 6, 91058 Erlangen, Germany

Liquid cell transmission electron microscopy (LCTEM) is a powerful technique to investigate chemical processes *in situ* on the nanoscale. Whilst commercial cell designs have the drawback that they need to be operated in a dedicated TEM holder and do not allow EDX analyses, we present an advanced design that overcomes these limitations and allows state-of-the-art *in situ* methods such as HRTEM, or EDXS.

Due to the chosen geometry, micropatterned wells in Si$_3$N$_4$ can be sealed with multi-layered graphene to bypass the shadowing effects in conventional micromachining-based liquid cells by simultaneously providing a defined cell volume. By exploiting these features, we demonstrate quantitative investigations of reaction kinetics of metal-based nanostructures and thus gain valuable insights into the underlying processes.

MM 20.12 Tue 18:30 Poster C

A new doping method for titanium oxide layers prepared by

plasma electrolytic oxidation — •Wolfram Gilbert, Mhamed El Achhab, and Klaus Schierbaum — Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany

Controlled doping procedures in semiconducting metal oxides are of general interest for the fabrication of mixed systems with n-type and p-type crystallites [1]. Plasma Electrolytic Oxidation (PEO) is a versatile technique to create titanium oxide gas sensing layers of different anatase/rutile ratios and microstructures [2]. To extend the technique to doped systems (e.g. p-type conducting TiO_2) we add chromium salts to the electrolyte during PEO and investigate the effect on the resulting phase composition and microstructure of the films.

For this purpose, oxide layers were formed on a 125 μm thick titanium foil under PEO conditions, using a 12.85 mol/l H_2SO_4 electrolyte, which was supplemented by $Cr_2(SO_4)_3$. In the experiments, the $Cr_2(SO_4)_3$ concentration of the electrolyte, electrostatic and potentiostatic components, voltage steps and maximum current strength were changed systematically. Size and morphology of the generated layers were measured in cross-section by SEM. Chromium in the sample was detected by EDX. The crystal structure was determined by XRD and Raman spectroscopy.

[1] Y. Li *et al.*, Sensors and Actuators B: Chemical **83** (1-3), S. 160-163 (2002)
[2] M. El Achhab and K. Schierbaum, J. Sens. Sens. Syst. **5**, 273 (2016)

MM 20.13   Tue 18:30   Poster C
Porous titanium oxide produced by plasma electrolytic oxidation in DC operation mode and various electrolyte concentrations — •Bernd Engelkamp, Mhamed El Achhab, and Klaus Schierbaum — Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany

Titanium oxide coatings produced by Plasma Electrolytic Oxidation (PEO) are of increasing scientific and commercial interest [1]. Prominent fields of applications are biomedical components and photocatalytic devices. Recent investigations revealed the potential for gas sensor technology [2]. The versatile character of PEO-produced coatings on titanium is due to the enormous scope of tailoring the coatings by using different process parameters. Many parameters serve as control levers, however, the most important are the electrical supply and the composition of the electrolyte. In our investigation we focus on the DC operation mode and the concentration of H_2SO_4 electrolyte [3]. We present layer thickness, porosity and phase composition (i.e. anatase and rutile ratio) of PEO-produced titanium oxide deduced from scanning electron microscopy, X-ray diffraction and Raman spectroscopy.

[1] T. W. Clyne and S. T. Troughton, Int. Mater. Rev. **63**, 1 (2018)
[2] M. El Achhab and K. Schierbaum, J. Sens. Sens. Syst. **5**, 273 (2016)
[3] B. Engelkamp *et al.*, Metals **8**, 386 (2018)

MM 20.14   Tue 18:30   Poster C
Structural phase transitions in palladium hydrogen thin films: Mechanical stress impact on critical temperatures — •Stefan Wagner and Astrid Pundt — Karlsruhe Institute of Technology, Institute of Applied Materials (IAM-WK), Karlsruhe, Germany

Palladium hydrogen (PdH) thin films serve as model systems to study structural phase transitions under elastic and microstructural confinements. Mechanical stresses linked to hydrogen-absorption of thin films clamped onto hard substrates are used to tune the hydrogens chemical potential, changing the stability of the hydride phase. Stresses are superimposed by microstructural constraints, channelling stress relaxation processes in the films. In-situ measurements of chemical potential and mechanical stress enable the determination of the attractive H-H interaction energy and of the critical temperature of hydride formation. Thereby partially relaxed stresses yield sloped plateaus in the two-phase-coexistence region, that need to be considered in the systems thermodynamic description [1]. [1] S. Wagner, A. Pundt, Int. J. Hydr. Energy 41 (2016) 2727.

MM 20.15   Tue 18:30   Poster C
Containment free in-situ analysis of gold nanorod growth using disposable 3D-printed experimental chambers — •Tobias Zech, Tilo Schmutzler, and Tobias Unruh — LKS, Friedrich-Alexander-Universität Erlangen-Nürnberg

Despite gold nanorods being used in various scientific fields, there still are some problems. Bad reproducibility, insufficient yield and time-consuming functionalization protocols are some of the burdens that

must be overcome. More systematic in-situ analyses using scattering techniques like small angle neutron and x-ray scattering would go a long way to get further insight into the anisotropic growth of gold nanorods. However, the chemical procedure always requires a clean and metal-ion free environment, to successfully produce gold nanorods. Also, the synthesis differs to a slight degree from synthesis to synthesis, which makes it hard to compare experiments with seemingly identical synthetic parameters on separately performed experiments. Therefore, we designed a cheap, compact, expendable experimental chamber using 3D-printing. This way, we were able to skip the possibly erroneous cleaning procedure and make systematic experiments over various synthetic parameters. 3D printing also gives us the flexibility of using different techniques like UV-Vis spectroscopy in parallel, to draw even more information out of our in-situ small angle scattering experiment. The chamber can be modified easily to include additional techniques like Raman and FTIR spectroscopy on the same sample volume in a containment free environment.

MM 20.16   Tue 18:30   Poster C
Interaction of polyamide 6 with galvanised steel and the influence of surface pretreatments — •Philipp Moritz[1,2], Lisa Wurlitzer[1,2], Maria Sonnenberg[1,2], and Wolfgang Maus-Friedrichs[1,2] — [1]Institute of Energy Research and Physical Technologies, Clausthal University of Technology, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — [2]Clausthal Centre of Material Technology, Clausthal University of Technology, Agricolastr. 2, 38678 Clausthal-Zellerfeld

Nowadays polymer-metal composites play a key role in the automotive and aerospace industry. The use of lightweight sandwich structures, for example, could lead to lower fuel consumption and decreasing CO_2 emissions. In order to improve the mechanical properties of these composites, the physical interaction of the layers is of particular interest.

We have produced composite materials from galvanised steel and polyamide 6 to investigate the bonding in more detail. In order to improve adhesion, the steel surface was additionally coated with a SiO_x layer using plasma-enhanced chemical solution deposition (PECSD). In further experiments, the effect of plasma-treated surfaces on the adhesion was investigated.

The adhesion behaviour was characterised by T-Peel tests and the exposed interfaces were studied with electron spectroscopy and microscopy. The spectroscopic analysis indicates different chemical bonds, due to the presence of the SiO_x layer.

MM 20.17   Tue 18:30   Poster C
Measurements of mechanical properties and microstructure on thin Cu based alloys — •Christian Aaron Rigoni, Martin Peterlechner, Harald Rösner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Germany

The mechanical properties of alloys are essential to industrial applications. Tensile testing is thus an appropriate material characterization technique. In general, such devices are bonded to certain sample dimensions as thickness and length. Thus measurements of microscale foils are a challenging task. An important point in this setup is the previous sample preparation since the sample cutting and finishing has a noticeable impact on the performance of the measurement. This effect was investigated in detail using wire erosion, punching, water and laser cutting. We analyse mechanical properties of thin Cu rich sheets with a thickness down to about 40 μm and a length of about 4 mm that were measured with a miniaturized tensile testing device. The goal is to obtain the dependence of the ultimate tensile strength and creep behavior in dependence of different temperatures with respect to the microstructure. A Norton-Bayley plot is obtained from the creep data in order to access the material constants and the results were discussed.

MM 20.18   Tue 18:30   Poster C
Tailoring the Microstructure and Electrochemical Behavior of Li-Mn-O Thin Film Battery Electrodes — •Henry Müller, Yug Joshi, Efi Hadjixenophontos, Claudia Peter, and Guido Schmitz — Institute of Materials Science, Chair for Materials Physics, University of Stuttgart, Heisenbergstraße 3, 70569 Stuttgart, Germany

Lithium manganese oxides have received great attention for application in lithium ion battery cathodes. In this complex ternary system, several compositions can be used to reversibly intercalate lithium. They crystallize in various structures ranging from different cubic across orthorhombic to monoclinic crystal systems. We use sputter deposition to manufacture high-capacity thin film electrodes with different compo-

sitions. In electrodes with a higher oxygen content the largest fraction of the material has a monoclinic crystal structure. Electrodes containing less oxygen crystallize mostly in rock salt and spinel structure. This can be used to tune the electrochemical behavior and capacity of the material by controlling the oxygen partial pressure during deposition.

MM 20.19   Tue 18:30   Poster C
Tuning the Energetic Landscape of Mixed Dimensionality Perovskites — •Haralds Abolins and Felix Deschler — Cavendish Laboratory, University of Cambridge, Cambridge, UK

Mixed dimensionality Ruddlesden-Popper perovskites have recently been shown to possess high performance in solar cells and greatly enhanced intrinsic stability relative to their bulk counterparts, which has proven the key challenge for the commercialization of perovskite-based photovoltaics. Nevertheless, the charge transport characteristics between the different phases in these materials have not been well understood. To elucidate the carrier dynamics in Ruddlesden-Popper perovskites a large single-phase grain system is developed and utilized to track the spatial distribution of the varying dimensionality domains in the resulting thin films and identify charge funnelling routes into the lowest band-gap phases of the material, which are shown to be tunable, as needed for specific applications.

MM 20.20   Tue 18:30   Poster C
TEM investigations of microstructure and manganese-valence evaluation in $Li_xMn_2O_4$ nanoparticles. — •Florian Schönewald, Max Baumung, Vladimir Roddatis, Marcel Risch, and Cynthia A. Volkert — Institut für Materialphysik, Georg-August Universität, Göttingen

Controlling the oxygen evolution reaction (OER) is an important step in achieving a sustainable renewable energy future. At the moment, the process of generating molecular oxygen from water by chemical means is severely kinetically limited. $Li_xMn_2O_4$ is studied here as a model electrocatalyst to understand the role of valence state and covalency on the electron transfer reaction.

The goal of this study is to control the OER by manipulating the manganese valence via electrochemical lithium de-/intercalation. Using TEM and STEM-EELS the structure and Mn valence of $Li_xMn_2O_4$-nanoparticles are investigated for different particle sizes and varying lithium content. Initial HR-TEM studies reveal no detectable changes in the particle surfaces as a result of lithiation cycles. In addition, TEM techniques are used to detect morphological changes in the active material after catalysing the oxygen evolution reaction with the aim to understand the underlying mechanisms.

MM 20.21   Tue 18:30   Poster C
Metal-insulator transition due to doping triggered localization — •Martin Hoffmann[1], Florian Sipek[1], Wolfram Hergert[2], and Arthur Ernst[1,3] — [1]Institute for Theoretical Physics, Johannes Kepler University Linz, Austria — [2]Institute of Physics, Martin Luther University Halle-Wittenberg, Germany — [3]Max Planck Institute of Microstructure Physics, Halle, Germany

Recent experiments found a doping induced metal-insulator transition (MIT) in $CaRu_{1-x}Co_xO_3$ at $x \approx 15\%$ [Adv. Sci. **5**, 1700978 (2018)], which was understood in terms of a simplified model as caused by Anderson localization. We are elaborating the idea of disorder induced localization using at first a tight-binding model for $CaRuO_3$ (CRO). The energy-level statistics of a direct diagonalized real-space clusters with randomly distributed Co impurities showed again hints pointing to localization. The latter reduces strongly the electron diffusion and, hence, causes the MIT. In order to support that model, we used also *ab initio* methods to study the electronic properties in Co doped CRO. The coherent potential approximation (CPA) within the Korringa-Kohn-Rostoker Green's function method (KKR-GF) allows the investigation of substitutional disorder. We observed strong variations in the density of states and the k-space energy landscape (Bloch spectral function) with increasing Co concentration – less s states and more d states appear at the Fermi energy. This result indicates as well the localization of electrons and a reduction of the electric current.

MM 20.22   Tue 18:30   Poster C
Electrochromism in Thin Film Lithium Ion Battery Electrodes — •Yug Joshi, Efi Hadjixenophontos, Juliane Mürter, Robert Lawitzki, and Guido Schmitz — Chair of Materials Physics, Institute of Material Science, University of Stuttgart, Stuttgart, Germany

Numerous lithium-ion battery electrodes have been studied for their electrochemical cyclabilty, reversibility, capacity. An interesting aspect of these electrodes, which has not gained much attention, is the change of optical properties upon dis-/charging (or electrochromism). In this study, we show the optical response of some well-known battery electrodes namely lithium manganese oxide (LMO), lithium iron phosphate (LFP), lithium cobalt oxide (LCO) and lithium titanate (LTO). The primary focus of this study is on the in-situ electrochromic characterization of the mentioned electrodes. The LMO and the LTO are further characterized ex-situ to calculate the refractive indices of the materials using the Clausius-Mossotti equation. This equation gives the electronic resonance wavelengths which are closely related to the band structure of the material. A particularly clear change in the resonance wavelength is observed upon de-/intercalation in LMO. For the LTO, since it is a phase-transformation based electrode, the optical constants in the dual phase region are represented as a combination of the pure phases, which yields information about the phase transformation mechanism. Finally, we consider options of utilizing these materials in optical integration based on silicon-based waveguides.

MM 20.23   Tue 18:30   Poster C
Microscopic Comosition Analysis of Transparent Conductive ZnO:Al — •Eric Weikum and Guido Schmitz — Chair of Material Physics, Institute of Materials Science, University of Stuttgart, Heisenbergstraße 3, 70569 Stuttgart, Germany

Transparent Conductive Oxides (TCO) are promising electrode materials for applications such as Light Emitting Devices and Photovoltaic. The state of the art TCO is Indium Tin Oxide, which suffers from its high cost. A possible alternative is Aluminum doped Zinc Oxide (ZnO:Al), which is studied in this work. The distribution of Aluminum Atoms is being studied using a Laser-Assisted Atom Probe, which allows chemical analysis on the nanometer scale. Tungsten tips are produced by Electropolishing and then developed using a Field Ion Microscope. These developed Tungsten tips are Sputter coated with Zinc Oxide, which is then Field Evaporated in a Laser-Assisted Atom Probe in order to obtain an atomic resolution of the chemical composition. The evaporation behavior of Zinc Oxide in High Electric Fields is being investigated at different doping concentrations and Laser intensities.

MM 20.24   Tue 18:30   Poster C
Template-Realized Functional Nanostructure Arrays for Electrical Energy Conversion and Storage — •Huaping Zhao, Long Liu, Yaoguo Fang, and Yong Lei — Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany

Functional nanostructures have gained wide concern in the contexts that rapid development of modern society raises huge requirements for modern and future devices. Facile realization of such nanostructures imposes a significant challenge for nanotechnology research and device applications. Template-based nanostructuring technique provides one promising approach to address this challenge owing to the superior geometrical characteristics of the templates. In particular, with perfectly-ordered porous anodic alumina membrane as template, perfectly-ordered nanostructure arrays of functional materials could be fabricated and are highly desirable for constructing high-performance energy devices. The functional nanostructure arrays with perfect periodicity stand as distinguished architectures thanks to their distinctive structural properties to tackle the primary challenges regarding the generation, transport and utilization of electrons, holes, ions or molecular species, etc. Therefore, functional nanostructure arrays have attracted intensive attention and yielded favorable electrochemical performance for energy conversion and storage.

MM 20.25   Tue 18:30   Poster C
LFP/Li3OCl/Si all solid state thin film battery — •Kun Zhang, Efi Hadjixenophontos, Yug Joshi, and Guido Schmitz — Chair of Materials Physics, Institute of Materials Science, University of Stuttgart, Heisenberg Straße 3, 705969 GERMANY

Due to the high energy density and excellent flame resistance of solid state batteries, the cruising range of vehicles could possibly be improved and the danger of spontaneous combustion avoided, if all-solid-state batteries become available. In this work, it is studied to which extent Li3OCl could be used as membrane in thin film all-solid-state batteries. Ion beam sputtering from a composite target of (Li2CO3+LiCl) give rise to smooth films of controlled thickness in the 100 nm to 500 nm range. The ionic conductivity is measured from RT up to 140

°C and the activation energy is evaluated to be equal to 0.57eV. A complete full battery is deposited by adding LFP and Si as thin film cathode and anode electrodes. The potential window and the capacity of the tri-layer system are investigated by Cyclic Voltammetry.

MM 20.26   Tue 18:30   Poster C

Ionic conductivity of LiBH4 molten films — •Efi Hadjixenophontos, Janina Trück, and Guido Schmitz — Heisenbergstrasse 3, 70569, University of Stuttgart, Institute of Materials Science, Departement of Materials Physics, Stuttgart, Germany

The fast Li ion conductivity in LiBH4 envisage its use as electrolyte in all solid state batteries. Whereas powders are commonly used, thin films provide a tool for examining the Li transport and learning more about such complicated systems. In this work films of LiBH4 are prepared by melting LiBH4 powder and their thickness is minimized by using spin coating. The two methods demonstrate reproducible thicknesses from 18.6 *m when flattened with a spatula and 5.3-1.3 *m depending on the rotation speed during spin coating. All layers are characterized by SEM for their thickness and by EDX and XPS for their composition. Though XPS investigations confirm the identification of the light elements composing LiBH4, EDX measurements reveal high oxygen quantities at the surface of the samples indicating the high sensitivity of the samples to air. The ionic conductivity is investigated by EIS and the change in the crystal structure is observed depending on temperature. The highest conductivity is achieved at 10-2 S/cm in the HT phase. Furthermore, the effect of different current collectors for improving the system is tested and Pt shows to improve the spin coating method.

MM 20.27   Tue 18:30   Poster C

Activation of methane and carbon dioxide by cationic tantalum clusters and their oxides under multi-collision conditions — •Theresa Zach, Nikita Levin, Jozef Lengyel, Martin Tschurl, and Ueli Heiz — Chair of Physical Chemistry, Department of Chemistry and Catalysis Research Center, Technical University of Munich, Lichtenbergstr. 4, 85748 Garching, Germany

The conversion of methane and carbon dioxide, potent greenhouse gases, to value-added products is considered as one the most desirable reactions in chemistry. Tantalum-based clusters exhibit promising properties on the activation of methane and carbon dioxide. The goal of our experiment is to investigate the complex reaction mechanisms using kinetic modeling in different size regimes, from the bare atom to clusters containing tens of atoms. Both reactions are measured experimentally in the gas-phase by ion trap mass spectrometry under multi-collisional conditions, which allow us to study the kinetics of the reactions as a function of temperature, which is essential to determine the corresponding activation energies. Using this setup for clusters of different sizes and oxidation states, we have surprisingly observed very promising catalytic activity of $[Ta_8O_2]^+$ in reaction with CH_4. The results suggest that the initial dehydrogenation of CH_4 to form $[Ta_8O_2CH_2]^+$ is in consecutive reaction with additional CH_4 yielding $[Ta_8O_2C_2H_6]^+$. $Ta_8O_2^+$ is then regenerated via release of the ethane. Further we intent to investigate the reactivity of Ta_n^+ clusters towards CO_2. The preliminary results of these experiments will be presented at the conference.

MM 20.28   Tue 18:30   Poster C

Tayloring morphology and carbon functionalization of LiFe$_x$Mn$_{1-x}$PO$_4$ — •Lennart Singer[1], Rouven Zeus[1], Enzo Moretti[1], Elisa Thauer[1], Peter Klar[2], Simon Burkhardt[2], Limei Chen[2], Michael Binnefeld[3], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute of Physics, Heidelberg University — [2]I.Institute of Physics, Justus-Liebig-University Gießen — [3]Institute of Pharmacy and Molecular Biotechnology, Heidelberg University

We report on the systematic variation of morphology, agglomeration and carbon functionalization in LiFe$_x$Mn$_{1-x}$PO$_4$ with various doping levels x and its effect on the electrochemical performance of the materials. A top-down approach applying a combination of solid-state synthesis and different post-treatment procedures such as ball milling, thermal treatment, and optical floating-zone purification is utilized to obtain pure materials with different primary particles size. Various mechanical and chemical approached to obtain appropriate carbon coating of the active material have been used. In addition, we also report a bottom-up microwave-assisted hydrothermal synthesis route where key parameters such as precursor concentration, additives, and pH-value of the reactant were varied to obtain materials of different size and agglomeration state.

MM 20.29   Tue 18:30   Poster C

ACuFe$_2$(VO$_4$)$_3$ (A = Li,Na) as cathode material for lithium-ion batteries — •Patrick Schilling[1], Yuquan Wu[1], Elisa Thauer[1], Alexander Vasiliev[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute of Physics, Heidelberg University, Germany — [2]Lomonosov Moscow State University, Moscow, Russia

ACuFe$_2$(VO$_4$)$_3$ (A = Li,Na) are novel mixed-spin chain materials which feasibility for application in lithium- and sodium-ion batteries bas been scarcely studied. Due to multiple transition metal ions (i.e., Cu^{2+}, Fe^{3+}, V^{5+}) providing potential redox centers, both materials are promising candidates for cathode materials in batteries. We report electrochemical studies vs. Na and Li, respectively. While no significant activity in a Na-battery is found for A = Na, LiCuFe$_2$(VO$_4$)$_3$ shows a clear redox pair centered at 2.5 V and several weaker features which we associate with V^{5+}/V^{4+} and V^{4+}/V^{3+}. Galvanostatic cycling shows continuous capacity decay from 270 mAhg^{-1} in cycle 2 to 180 mAhg^{-1} in cycle 10. XRD of electrodes at various stages of charging suggests the possible reversible formation of LiFeO$_2$ during lithium intercalation.

MM 20.30   Tue 18:30   Poster C

Water Adsorbtion on CuO$_x$ and NiO$_x$ clusters Attached to the Anatase TiO$_2$(101) Surface by DFT Calculations — •Leila Kalantari, Jasmin S. Schubert, Alexey Cherevan, Dominik Eder, and Peter Blaha — Institue of Materials Chemistry, Vienna University of Technology. Getreidemarkt 9/165-TC, A-1060 Vienna, Austria

Experimental studies have shown the possible production of hydrogen through photocatalytic water splitting using metal oxides (CuO$_x$ and NiO$_x$) attached on anatase TiO$_2$ nanoparticles. In this work, we performed density functional theory calculation to provide a detailed description of geometry, electronic properties, catalytic site and adsorption of water on Ni$_n$O$_n$ ($n = 0-6$) and Cu$_m$O$_n$($m = 1-6, n = 0-3$) attached to the anatase TiO$_2$(101) surface. The adsorption of Ni$_n$O$_n$ and Cu$_m$O$_n$ clusters on the TiO$_2$(101) surface has been studied using PBEsol exchange correlation functional with and without Hubbard correction (U). Various geometries of Ni$_n$O$_n$ and Cu$_m$O$_n$ have been investigated. It is found that the adsorption of a Ni atom on anatase TiO$_2$(101) surface is stronger than of Cu atom. Energetically, the NiO cluster prefers the bridge site oxygen atoms with an adsorption energy of 7.09 eV. We found that the Ni$_n$O$_n$ and Cu$_m$O$_n$ cluster adsorption energy remains about constant with cluster size which makes the formation of bigger cluster plausible as confirmed by TEM images. Water adsorbs non-dissociatively on the anatase (101) surface with an adsorption energy of 660 meV while water molecules dissociate on Cu$_2$O and metallic Cu attached to the anatase TiO$_2$(101) surface.

MM 20.31   Tue 18:30   Poster C

Enhancing photocatalytic efficiency of substoichiometric TiO$_x$ at visible wavelengths using nano-resonators with anapole modes — •Ludwig Hüttenhofer[1], Felix Eckmann[2], Javier Cambiasso[3], Evangelina Pensa[3], Yi Li[1], Emiliano Cortés[1,3], Ian D. Sharp[2], and Stefan A. Maier[1,3] — [1]Nanoinstitut Ludwig-Maximilinas-Universität, Königinstraße 10, 80539 München, Germany — [2]Walter-Schottky-Institut Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany — [3]Centre for Plasmonics and Metamaterials Imperial College, 180 Queen's Gate, SW7 2AZ London, United Kingdom

TiO$_2$ has been shown to be a good candidate as photocatalyst also allowing for for water splitting. On the other hand the semiconductors band gap only harvests the small UV portion of the solar spectrum. To permanently turn the material absorptive in the visible spectral range the material is annealed at vacuum. This induces oxygen vacancies in the TiO$_2$ giving rise to sub-bandgap states (OV-TiO$_2$). In this work we shape OV-TiO$_2$ into nano-disks exhibiting anapole resonances. This mode is characterized by a minimum if its far-field scattering and a maximum of electric energy inside the resonator. The goal of this work is to show that by varying the nano-disk geometry we can spectrally locate the anapole resonance within the oxygen vacancy states and therefore maximize the absorption. As a proof of concept study we want to demonstrate the exploitation of anapole modes by the preferred reduction of Ag on the resonant disks surface under 532nm laser excitation on a single particle level.

MM 20.32   Tue 18:30   Poster C

Thermal conduction in epitaxial LaMnO3/SrMnO3 super-lattices — •Daniel Metternich[1], Dennis Meyer[1], Roland

POTTHAST[1], JAN-PHILLIP BANGE[1], MARIUS KEUNECKE[1], VLADIMIR RODDATIS[2], VASILY MOSHNYAGA[1], and HENNING ULRICHS[1] — [1]I. Physikalisches Institut, Georg-August Universität Göttingen, Germany — [2]Institut für Materialphysik, Georg-August Universität Göttingen, Germany

We report on our experimental investigations of the thermal conduction in LaMmO$_3$ (LMO) / SrMnO$_3$ (SMO) epitaxial superlattice structures, grown by metal-organic aerosol deposition (MAD).

The thermal conductivity of our samples is measured with a transient thermoreflectivity setup - a method that uses a pulsed laser to heat the sample whilst a continuous wave laser measures the surface reflectivity (TTR), and thereby the surface temperature in the time domain. We show that TTR is optimally suited for our oxide samples, which feature rather slow thermal dynamics. We elucidate the influence of different periodicities and arrangements of the layers of the superlattice. Furthermore, the thermal conductivity of the superlattice structures are compared to homogeneous LSMO, LMO, and SMO films. This in particular enables us to study the effect of the interfaces between LMO and SMO. Given the high structural quality of our superlattice, we also briefly discuss our plans to compare our findings with theoretical modelling and ultimately with first-principles calculations of phonon band structures. We acknowlegde financial support by the DFG within SFB1073.

MM 20.33 Tue 18:30 Poster C

Nanoporous gold as carrier for electrochemically assisted immobilization of redox-active enzyme using a cationic binding module — ●ELISABETH HENGGE[1], EVA-MARIA STEYSKAL[1], ALEXANDER DENNIG[2], BERND NIDETZKY[2], and ROLAND WÜRSCHUM[1] — [1]Inst. of Mater. Phys., TU Graz — [2]Inst. of Biotechnol. and Biochem. Eng. , TU Graz

An attractive application of nanoporous metals is in the field of biocatalysis, among which an important issue is related to the immobilization of enzymes that catalyse redox reactions. Here, we combine tailor-made enzymes with a nanoporous metal electrode under electrochemical control to enable regulation of the binding mechanisms and in-situ monitoring of underlying kinetics. An AuAg master alloy was used to produce self-supporting nanoporous gold samples by dealloying [3]. The pore size was optimized for immobilization by thermal annealing. As enzyme, the cytochrome P450 BM3 [2] fused to Z$_{Basic2}$ has been chosen. It is already known that this binding module provides the possibility for oriented and selective immobilization on non-metallic carriers [1]. The influence of the surface charge on the immobilization is studied in-situ in an electrochemical cell. Simultaneously, we determine the decrease of enzyme concentration in the electrolyte by UV/VIS spectroscopy. The biocatalytic activity of this new hybrid material was investigated by using lauric acid as a model substrate. [1] Bolivar JM, Nidetzky B, Langmuir 28 (2012) 10040. [2] Valikhani D et al. Biotechnol. Bioeng. 115 (2018) 2416. [3] Steyskal EM et al. Phys. Chem. Chem. Phys. 19 (2017) 29880.

MM 20.34 Tue 18:30 Poster C

Optimization and characterization of rf sputtered LiCoO2 cathodes — ●MARCEL COUTURIER, FABIAN MICHEL, MARTIN BECKER, and ANGELIKA POLITY — Institute for Exp. Physics I and Center for Materials Research (LaMa), Justus Liebig University Giessen, Germany

LiCoO$_2$ (LCO) thin films have been grown by rf-magnetron sputter-deposition on platinum-coated Al$_2$O$_3$ (c-sapphire) substrates. Deposition parameters such as substrate temperature and the partial pressure ratio between O$_2$ and Ar were varied in order to find suitable parame-

ters for a cathode offering reversible intercalation and deintercalation of lithium ions. Structural characterization was carried out using X-ray diffraction and Raman spectroscopy, revealing that the orientation as well as the crystallinity of the deposited LiCoO$_2$ films can be influenced by varying the O$_2$/Ar-ratio and simultaneously applying a sufficient substrate temperature during deposition. Furthermore, both the atomic composition and the atomic distribution were determined using X-ray photoelectron spectroscopy and secondary ion mass spectrometry. Results showed that the films are nearly stoichiometric and have a homogeneous atomic distribution throughout the entire depth profile. For electrochemical characterization, LiCoO$_2$ thin films where charged and discharged against lithium metal while using a liquid electrolyte consisting of LiPF$_6$ dissolved in a mixture of EC/DMC with a molar fraction of 1:1. Reversible discharge capacities in the order of up to 70 mAh/g could be achieved for optimized LiCoO$_2$ thin films.

MM 20.35 Tue 18:30 Poster C

Development of a Neural Network Potential for Metal-organic Frameworks — ●MARIUS HERBOLD, MARCO ECKHOFF, and JÖRG BEHLER — Georg-August Universität Göttingen, Institut für Physikalische Chemie, Theoretische Chemie, Tammannstraße 6, 37077 Göttingen, Germany

Metal-organic frameworks (MOFs) are porous crystalline materials with many applications in chemistry and materials science, from gas separation to heterogeneous catalysis. To date, computer simulations of chemical processes in MOFs are severely limited by the use of classical force fields, which in most cases are unable to describe the making and breaking of bonds. Electronic structure methods like density-functional theory (DFT) in principle offer a solution for this problem, but often the required systems are too large for routine applications of DFT. Here we present a high-dimensional neural network potential for a series of MOFs, which combines the accuracy of first principles with the efficiency of simple empirical potentials. We demonstrate that it is possible to obtain a reliable description of the potential-energy surface based on reference calculations of molecular fragments only.

MM 20.36 Tue 18:30 Poster C

In Situ Impedance Analysis of LSC Thin Films during Growth on YSZ and LSGM — ●MATTHÄUS SIEBENHOFER, GHISLAIN M. RUPP, JÜRGEN FLEIG, and MARKUS KUBICEK — Institute of Chemical Technologies and Analytics, Vienna University of Technology

The mixed conducting perovskite material La$_{0.6}$Sr$_{0.4}$CoO$_{3-\delta}$ (LSC) is a very promising cathode material for application in a solid oxide fuel cell (SOFC) due to its catalytic properties for the oxygen surface exchange and its high electronic conductivity. A factor which is essential to consider in the characterization of LSC is the influence of lattice strain on the surface exchange resistance and the chemical capacitance. Recent findings showed that tensile strained films exhibit faster surface exchange and diffusion compared to compressively strained films.

In this study the influence of the two different substrates Y$_2$O$_3$:ZrO$_2$ and (La,Sr)(Ga,Mg)O$_3$ on LSC thin films was examined with a novel method allowing in situ impedance spectroscopy during the PLD process (IPLD). That way, it is possible to track charge carrier densities during growth and to link the results with microstructure and strain.

According to the measurements, tensile strain leads to an increase of the chemical capacitance by a factor of 1.6 and therefore to an increase of the effective concentration of oxygen vacancies. Furthermore a decrease of the surface exchange resistance by 50 % was observed. These results are also in agreement with previous theoretical studies which suggest that tensile in-plane lattice strain lowers the vacancy formation energy and therefore increases the vacancy concentration.

MM 21: Invited talk Chen

Time: Wednesday 9:30–10:00   Location: H43

Invited Talk   MM 21.1   Wed 9:30   H43
Rational design of Cu based shape memory alloys with low functional fatigue properties — •Xian Chen and Mostafa Karami — Hong Kong University of Science and Technology, Hong Kong

Discoveries and optimization of novel properties of materials underlie the advanced technologies that greatly improve the quality of our modern life. Our engineering heuristics usually guide the discovery of new

materials, but the transitioning of the property from the initial discovery to the optimized one for practical use usually takes more than a decade. In fact, these engineering optimization problems should be under the umbrella of "Mathematics". In this talk, we will introduce a theory-based alloy development method for shape memory alloys. We exploit the synergy of the theories, the suite of algorithms and the advanced characterizations to develop Cu-based shape memory alloys with optimized functional fatigue properties.

MM 22: Materials for Energy Storage and Conversion

Sessions: Computational I and II

Time: Wednesday 10:15–13:15   Location: H43

MM 22.1   Wed 10:15   H43
First-Principles Calculations of Charge States in Defective SOFC/SOEC Perovskite Materials — •Daniel Mutter[1], Daniel F. Urban[1], and Christian Elsässer[1,2] — [1]Fraunhofer IWM, Wöhlerstraße 11, 79108 Freiburg — [2]Freiburger Materialforschungszentrum FMF, Stefan-Meier-Str. 21, 79104 Freiburg

Solid oxide fuel cells (SOFC) and solid oxide electrolyzer cells (SOEC), which transform chemical into electrical energy and vice versa, have the potential to make a significant contribution to the efforts of overcoming future problems of the energy economy. An optimal functionality of these devices requires a high catalytic activity at the electrodes. This strongly depends on point defect concentrations and on the capability of the material to allow for fast charge transfer reactions. Promising anode materials regarding these requirements are perovskite compounds (ABO_3), where the transition-metal ion on the B site can adopt different oxidation states by accepting and releasing electrons during the oxygen reactions at the SOEC/SOFC surfaces. We present results of density functional theory GGA+U calculations for the changes in oxidation states of the transition metal ions Fe and Mn in $LaFeO_3$ and $La_xCa_{1-x}MnO_3$ ($0 \leq x \leq 1$), respectively, when point defects such as anionic and cationic vacancies are present near the metal ions. After identifying the dominant defect species, a Bader charge analysis was performed and partial electronic densities of states were derived. The latter are compared to electron energy-loss near-edge spectra (ELNES), which are sensitive to changes of the bonding environment and hence of the oxidation states of individual atoms.

MM 22.2   Wed 10:30   H43
Interaction of the H_2 molecule with carbon nanostructures: A DFT study — •Dominik Nöger and David Holec — Department of Materials Science, Montanuniversität Leoben, Franz-Josef-Strasse 18, A-8700 Leoben, Austria

On a long path of finding appropriate materials to store hydrogen, graphene and carbon nanotubes have drawn a lot of attention as potential storage materials. Their advantages lie at hand since those materials provide a large surface area (which can be used for physisorption), are cheap compared to metal hydrides, are abundant nearly everywhere, and most importantly, can increase safety to existing storage solutions. The present Density Functional Theory (DFT) study employs Tkatchenko-Schäffler (TS) van-der-Waals correction. The preferred adsorption site for an H_2 molecule is the hollow (centre of hexagon) site of planar graphene, with the molecule orientated parallel to graphene. Next, the influence of vacancy and Stone-Wales defects in graphene was studied. Neither of them provides increased adsorption energies for H_2. Interestingly, vacancy shows a capability to capture H_2 inside the defect in a metastable state; this configuration is unstable both for pure graphene as well as for the Stone-Wales defect. Finally, the impact of different carbon nanotube diameters and geometries (zigzag & armchair configuration) on physisorption energetics and behaviour is presented.

MM 22.3   Wed 10:45   H43
6Mg(NH2)/9LiH/LiBH4: Molecular Dynamics and Hydrogen Diffusion — •Neslihan Aslan[1,2], Wiebke Lohstroh[2], Sebastian Busch[1], Claudio Pistidda[1], Klaus Pranzas[1], and Mar-

tin Müller[1] — [1]Helmholtz-Zentrum Geesthacht, Germany — [2]Heinz Maier-Leibnitz Zentrum, TUM, Garching, Germany

Methods to store hydrogen are e.g. physical technologies (compression) or chemical bonding in metal hydrides. Within the complex hydrides, the metal amides Mg(NH2)2-LiH have recently gained in importance. They have good hydrogen storage properties with high capacity (ca. 4 wt%) and good reversibility. The drawback of these materials is the high kinetic barrier for hydrogenation, which results in a long loading time. This can be overcome with the addition of LiBH4. So far Mg(NH2)2-LiH-LiBH4 is an outstanding candidate for hydrogen storage. Interestingly, some compositions can even reach operation temperatures below 100 °C and the desorbed products contain amongst others liquid phases. The hydrogen uptake and release properties of this system are well characterized in terms of capacity, kinetics and phase composition, but the basic mechanism how the reaction takes place and why it has these excellent storage facilities is still unknown. With 6Mg(NH2)/9LiH/LiBH4 we want to understand the system and the reaction mechanism. We will present first data of neutron scattering experiment using quasielastic scattering at TOFTOF to study hydrogen diffusion of the desorbed and absorbed state, as well as small angle neutron scattering to study particle sizes to gain further insight on the hydrogenation/dehydrogenation mechanism.

MM 22.4   Wed 11:00   H43
Applicability of MAX phases as diffusion barrier for hydrogen and chromium in SOFC — •Daniel F. Urban[1,2], Dimitrios Satkas[1], and Christian Elsässer[1,2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]University of Freiburg, FMF, Germany

Promising candidates in the search for corrosion protection coatings for high temperature energy-conversion devices such as solid oxide fuel cells (SOFC) are MAX phases which are ternary metal carbides and nitrides with multi-layered crystal structures. To assess the capability of MAX phases as diffusion barriers for hydrogen and chromium, we investigate the absorption and migration of H and Cr atoms in a variety of MAX-phase carbides and nitrides by means of first-principles calculations based on density functional theory. Based on the calculated formation and migration energies we discuss how MAX-phase coatings can act as efficient protective diffusion barriers for both hydrogen and chromium and explain the underlying migration mechanisms. While Cr atoms are found to diffuse via a vacancy mediated mechanism and substitute M- and A-atoms, H diffusion occurs on essentially decoupled bilayer dice-lattices of tetrahedrally and octahedrally coordinated interstitial sites. [1]. We discuss the possibility to tailor specific material properties like lattice constants or thermal expansion coefficients for a given required diffusion barrier impact by making use of the flexibility of the MAX-crystal structure which allows for mixed $(M_1,M_2)(A_1A_2)X$ phases.
[1] F. Colonna, C. Elsässer, RSC Advances 7, 37852 (2017).

MM 22.5   Wed 11:15   H43
Description of bulk and surface polarons in oxide materials using DFT+U — •Matthias Kick, Cristina Grosu, Christoph Scheurer, Karsten Reuter, and Harald Oberhofer — Technische Universität München

Lithium titanium oxide $Li_4Ti_5O_{12}$ (LTO) is an intriguing anode ma-

terial promising particularly long lived batteries, due to its remarkable phase stability during (dis)charging of the cell. Moreover, its high intercalation potential also prevents the formation of Li dendrites. Unfortunately, the low intrinsic electronic conductivity of LTO still severely limits its use. An elegant way to improve on this drawback, is to introduce oxygen vacancies resulting in formation of Ti^{3+} centers. In our study we use *Hubbard corrected density-functional theory* (DFT+U) to show that this leads to the formation of polaronic states, which can again hamper electron conduction. In order to gauge the polaronic charge mobility we compare the relative stabilities of different polaron location patterns in bulk and surface LTO for a number of oxygen defects.

15 min. break

MM 22.6   Wed 11:45   H43

Solid-State Li_2S-P_2S_5 Electrolytes: A DFT based Force-Field Parameterization — •Carsten Staacke[1], Simon Rittmeyer[1], Hendrik Heenen[1], Johannes Voss[2], Christoph Scheurer[1], Alan Luntz[2], and Karsten Reuter[1] — [1]Theoretische Chemie, TU München — [2]SLAC National Accelerator Laboratory, USA

All-solid-state Li-ion batteries promise gains in safety and durability by replacing the liquid by a solid-state electrolyte (SSE). In this context, the xLi_2S-(100-x)P_2S_5 (LPS) SSE group, especially $Li_7P_3S_{11}$, has gained much attention. While $Li_7P_3S_{11}$ glass has a rather limited conductivity, a meta stable glass-ceramic state shows impressive conductivity [1]. Understanding the reasons for this large change of conductivity, requires a detailed atomistic description not directly accessible from experiment. On the other hand, the material complexity and timescales involved in realistic glass-ceramic SSE simulations are beyond current predictive-quality density-functional theory (DFT) based molecular dynamics. We therefore engage in the development and first-principles validation of a polarizable force field for the LPS SSE. In particular, the Buckingham parametrization and polyanion models are discussed. We further give a perspective on how to improve our scheme by Gaussian approximation potentials (GAP).
[1] A. Hayashi, A. Sakuda, M. Tatsumisago, *Front. Energy Res.*, **2016**, *4*, 25

MM 22.7   Wed 12:00   H43

Elastic moduli of LISICON and garnet superionics from first-principles molecular dynamics variable cell — •Giuliana Materzanini and Nicola Marzari — Theory and Simulation of Materials (THEOS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

In this work we have calculated elastic moduli of different materials belonging to two of the most studied and most performing families of crystalline ionic conductors, namely the LISICONs and the garnets, LGPS ($Li_{10}GeP_2S_{12}$), LGPO ($Li_{10}GeP_2O_{12}$) and LLZO ($Li_7La_3Zr_2O_{12}$), in their different phases. Sampling of the space-phase was performed according to Car-Parrinello molecular dynamics in the variable cell volume and shape NpT ensemble. From the MD trajectories the time-dependent cell and strain matrices were extracted and the strain fluctuations were calculated as block averages of the strain tensor cross-products, for which statistical convergence was carefully monitored. Results for the elastic moduli of the different materials and for their different phases were reported and discussed, on the light of the available experimental literature.

MM 22.8   Wed 12:15   H43

Cage-hopping mechanism of lithium cation diffusion in liquid thiophene-derivatives as revealed by AIMD simulations — •Pouya Partovi-Azar and Daniel Sebastiani — Martin-Luther Universität Halle-Wittenberg

Unraveling the diffusion mechanism of Li^+ in thiophene-based liquids is of great importance in reaching optimal electrolyte compositions for Li-based energy-storage devices. However, the dynamics of Li^+ in thiophene-based electrolytes is barely known at an atomistic level, which makes it hard to reveal the actual mechanism of the diffusion. Here, we report on DFT-based *ab initio* molecular dynamics simulations performed to study the fundamental processes occurring in the Li^+/thiophene-based systems. We consider Li^+ ions at 1M concentration in thiophene and 3,4-ethylenedioxythiophene (EDOT) liquids in the condensed phase. Our simulations reveal a cage-hopping mechanism for Li^+ diffusion in both liquids. Each Li^+ is surrounded by four liquid molecules in a cage structure, while being coordinated by four sulfur and four oxygen atoms in the case of thiophene and EDOT, respectively. The liquid molecules in a cage form a slightly deformed tetrahedron, where a "weak" part is formed due to repulsive interaction between two closer sulfur atoms, allowing the Li^+ ion to escape the cage. This finding can be directly used to define proper collective variables for metadynamics or kinetic Monte-Carlo simulations. The thermal energy at 300K is found to be enough to trigger a Li^+ hopping in the thiophene liquid, but falls short in the case of EDOT liquid, which possesses a stronger molecular network due to H bonding.

MM 22.9   Wed 12:30   H43

Dense storage of alkali metals between graphene bilayers: a computational study — •Mahdi Ghorbani-Asl[1], Ilia Chepkasov[1,2], and Arkady V. Krasheninnikov[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Katanov Khakass State University, pr. Lenina 90, Abakan 655017, Russia

We study the intercalation of alkali metals, namely lithium and sodium, between graphene sheets using density functional theory calculations with the van der Waals correction. The structures and energetics of a different number of alkali layers with closed packed structure have been investigated for AB and AA stacking sequences of bilayer graphene. The intercalation energies suggested that the AA stacking is more favorable for the single-layer intercalation but it has less effect on the multilayered storage. Our calculations showed that there is a clear correlation between the intercalation energy and the electron transfer between the intercalate and graphene. While the higher values of charge transfer observed for the single layer intercalation, the charge transfer is noticeable only for the outer alkali layers in the multi-layer case. As a result, the intercalation energy reduces with increasing the number of the layer from double to triple layers. The present study can shed light on the design of high storage alkali batteries using two-dimensional layered materials as reported recently [1].
[1] M. Kühne, F. Börrnert, S. Fecher, M. Ghorbani-Asl, J. Biskupek, D. Samuelis, A. V. Krasheninnikov, U. Kaiser, J. H. Smet, Nature (2018). https://doi.org/10.1038/s41586-018-0754-2

MM 22.10   Wed 12:45   H43

A first-principles based LATP force-field for grain-boundary simulations — Simon Rittmeyer[1], Karsten Reuter[1], Rüdiger Eichel[2], and •Christoph Scheurer[1] — [1]Theoretische Chemie, TU München — [2]IEK-9, FZ Jülich

Superionic lithium-ion conductors of NASICON structure are promising solid-state electrolytes (SSE) for all solid-state batteries (ASSB). A detailed multi-modal experimental analysis of carefully sintered $Li_{1+x}Al_xTi_{2-x}(PO_4)_3$ (LATP, $x = 0.3$) has yielded interesting structural insights and a surprisingly lower ionic conductivity in the amorphous grain boundary interphase than in the grain bulk.[1] Combined with high cycling stability observed in a LATP-based phosphate-backbone ASSB, these findings call for a detailed microscopic understanding. We have constructed a first-principles based force-field which covers stoichiometries $x = 0 \ldots 0.3$ and sampled surface slab models representing possible LATP mixed occupancies. DFT computations on large surface models yield first insights into the mechanisms behind the peculiar properties of this material.
[1] A. Mertens, S. Yu, N. Schön, D. Guenduez, H. Tempel, R. Schierholz, F. Hausen, H. Kungl, J. Granwehr, and R. Eichel, Solid state ionics **309** (2017), 180.

MM 22.11   Wed 13:00   H43

Effect of mixed surface terminations on the structural and electrochemical properties of two-dimensional $Ti_3C_2T_2$ and V_2CT_2 MXenes multilayers — •Nuala Mai Caffrey — School of Physics & CRANN, Trinity College, Dublin 2

MXenes, a family of layered transition metal carbides and nitrides, have shown great promise for use in emerging electrochemical energy storage devices, including batteries and supercapacitors [1]. However, MXene surfaces are terminated by randomly distributed –O, –F and –OH functional groups and there is considerable debate regarding how the intercalating alkali metal ions interact with these functional groups. For instance, their measured Li or Na capacity is far lower than that predicted by theoretical simulations, which generally assume uniformly terminated surfaces. The extent to which this structural simplification contributes to such discrepancies is unknown.

I address this issue by employing first-principles calculations to compare the structural, electronic and electrochemical properties of two

common MXenes, namely $Ti_3C_2T_2$ and V_2CT_2, with both uniform terminating groups and explicitly mixed terminations [2]. I find that the redox reaction is confined to the terminating groups for low concentrations of intercalated metal ions, with the oxidation state of the metal atoms unaffected until higher concentrations are achieved, in excellent agreement with experiment.

[1] Anasori et al, Nature Reviews Materials **2** 16098 (2017)
[2] Caffrey, Nanoscale **10** 13520 (2018)

MM 23: Methods in Computational Materials Modelling (methodological aspects, numerics)

Sessions: APT and Diffusion; Method and Code Development

Time: Wednesday 10:15–13:15   Location: H44

MM 23.1   Wed 10:15   H44
Understanding field evaporation in atom probe tomography from a first-principles perspective — •Christoph Freysoldt, Michael Ashton, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40273 Düsseldorf

Field evaporation is the elementary process at the heart of atom probe tomography (APT): single atoms or molecules evaporate from the sample under the influence of a very high electric field. Despite 50 years of APT experiments, a comprehensive predictive theory is still lacking.

We approach the problem in the framework of density-functional theory. From the minimum-energy path for desorption as a function of applied field, we compute critical fields and transition barriers for a variety of surface sites in good agreement with available experimental data. Our results show that atoms evaporating from within the surface at steps or kinks stay in close bonding contact at the transition state. The surface bonding characteristics of the evaporating atom is thus much more important than the electron transfer process, which was assumed to be the dominant mechanism in previous models.

From our insights, we propose a simple analytic theory. The critical zero-barrier field results from the balance between the maximum intrinsic force along the reaction coordinate and the field-induced force. The latter can be obtained directly from the change of the surface dipole along the reaction coordinate, while the former is not very sensitive to the applied field. The theory also provides barrier heights for subcritical fields.

MM 23.2   Wed 10:30   H44
Evaporation Mechanisms for Field-Ionized Surface Atoms — •Michael Ashton, Christoph Freysoldt, and Joerg Neugebauer — Max Planck Institut für Eisenforschung GmbH, Max-Planck-Str. 1 40273 Düsseldorf

Detailed information regarding the atomic-scale mechanisms of field evaporation has long eluded the theoretical community, in part due to the challenge of applying finite electric fields in density functional theory (DFT) models that require periodic boundary conditions. We explain how our recent advances in the treatment of electric fields in DFT have enabled fundamental insights into the near-surface mechanisms of field evaporation for atoms on Tungsten surfaces. These insights are obtained from static calculations of the energy landscapes for low-coordinated atoms departing from a charged surface. They show that even for very strong fields a two-stage rollover mechanism - in which an evaporating kink atom rolls into the hollow site above the neighboring step and then proceeds to evaporate - is the minimum energy path. We find that this two-stage rollover mechanism is circumvented at fields very close to the critical evaporation field, resulting in a much simpler single barrier trajectory. The origin of this change in mechanism will be discussed along with some of its implications for experimental evaporation procedures. Finally, we discuss the similarities and differences between our DFT results and those obtained using classical models to describe field evaporation.

MM 23.3   Wed 10:45   H44
Atomistic description of self-diffusion in molybdenum — Daria Smirnova[1], Yanyan Liang[1], Grisell Diaz Leines[1], Sergei Starikov[1], Ning Wang[1], •Matous Mrovec[1], Ralf Drautz[1], Davide Sangiovanni[2], Igor Abrikosov[2], and Maxim Popov[3] — [1]The Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Germany — [2]Linköping University, Linköping, Sweden — [3]Materials Center Leoben Forschung GmbH, Leoben, Austria

According to the experimental data, self-diffusion coefficient in molybdenum shows non-Arrhenius behavior, however, its origin is controversial. In this work, we apply first-principle calculations and classical molecular dynamics to study the nature of self-diffusion in bcc molybdenum. We consider vacancy diffusivities, formation and migration energies depending on temperature in a wide temperature range: from zero temperature up to the melting point. We also carried out molecular dynamics simulations that allow to observe directly the process of self-diffusion at the atomic scale. Summarizing the results obtained by different calculation methods, we can conclude that the peculiarity observed for self-diffusion can be caused by strong temperature dependence of the vacancy formation energy. The methodology reported here is universal and can be applied to analyze self-diffusion in another metals.

MM 23.4   Wed 11:00   H44
The Anharmonicity of Al self-diffusion — Raynol Dsouza, •Liam Huber, Blazej Grabowski, and Joerg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

To study kinetic properties, e.g. diffusion, at the atomistic scale with molecular dynamics (MD) it is usually necessary to operate at very high temperatures where processes occur at high rates, or to use some approximation or acceleration scheme. At low temperatures it is common to use the quasi-harmonic approximation (QHA), where finite-T effects are represented using phonon calculations. However, even for the relatively simple thermodynamic property of vacancy formation in aluminum, anharmonic effects not captured by QHA appear well below room temperature [1].

In this work, we apply the finite temperature string method [2] to study the effect of these anharmonicities on Al self-diffusion. This technique allows us to probe the temperature range above the threshold at which QHA begins to lose validity, but still well below the temperature at which calculation by direct MD becomes feasible. Finally, we consider the combination of thermodynamic integration [3] with FTS in order to capture anharmonic behaviour with the full power and accuracy of quantum mechanics.

[1] Glensk et al. Phys Rev X 4 (2014)
[2] Vanden-Eijnden and Venturoli, J Chem Phys 130 (2009)
[3] Duff et al. Phys Rev B 91 (2015)

MM 23.5   Wed 11:15   H44
Kinetic Monte Carlo simulations of vacancy diffusion in non-dilute Ni-X (X=Re,W,Ta) alloys — •Maximilian Grabowski, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, 44801 Bochum, Deutschland

The mobility of vacancies in alloys may limit dislocation climb which is important for high performance Ni-based superalloys. Using a combined density functional theory and kinetic Monte Carlo approach we investigate vacancy diffusion in Ni-Re, Ni-W, and Ni-Ta binary alloys up to 10 at.% solute concentration. We introduce an interaction model that takes into account the chemical environment close to the diffusing atom to capture the effect of solute-host and solute-solute interactions on the diffusion barriers. In contrast to an ideal solid solution it is not only the diffusion barrier of the solute atom that influences the vacancy mobility, but primarily the change in the host diffusion barriers due to the presence of solute atoms. This is evidenced by the fact that the observed vacancy slowdown as a function of solute concentration is larger in Ni-W than in Ni-Re, even though Re is a slower diffuser than W. To model diffusion in complex, non-dilute alloys an explicit treatment of interaction energies is thus unavoidable. In the context of Ni-based superalloys two conclusions can be drawn from our kinetic Monte Carlo simulations: the observed slowdown in vacancy mobility is not sufficient to be the sole cause for the so-called Re-effect; and assuming a direct correlation between vacancy mobility, dislocation climb, and creep strength the experimentally observed similar effect of W and Re in enhancing creep strength can be confirmed.

15 min. break

MM 23.6   Wed 11:45   H44

Density-gradient-free variable in exchange-correlation functionals for detecting inhomogeneities in the electron density — •Fabien Tran and Peter Blaha — Vienna University of Technology, Vienna, Austria

A new type of approximation for the exchange and correlation functional in density functional theory is proposed. This approximation depends on a variable, u, that is able to detect inhomogeneities in the electron density ρ without using derivatives of ρ. Instead, u depends on the orbital energies which can also be used to measure how a system differs from the homogeneous electron gas. Starting from the functional of Perdew, Burke, and Ernzerhof (PBE) [Phys. Rev. Lett. **77**, 3865 (1996)], a functional depending on u is constructed. Tests on the lattice constant, bulk modulus, and cohesive energy of solids show that this new u-dependent PBE-like functional is on average as accurate as the original PBE or its solid-state version PBEsol. Since u carries more nonlocality than the reduced density gradient s used in functionals of the generalized gradient approximation (GGA) like PBE and α used in meta-GGAs, it will be certainly useful for the future development of more accurate exchange-correlation functionals.

MM 23.7   Wed 12:00   H44

Advanced Path Integral Methods - Beyond the Benchmarks — •Venkat Kapil and Michele Ceriotti — Institute of Materials,Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

The precise description of quantum nuclear fluctuations in atomistic simulations is possible by employing path integral techniques. However, many challenges such as the high computational cost of running path integral simulations and the overhead of implementation of path integral methods in electronic structure packages, have prevented their widespread use. In this talk, I will present molecular dynamics (MD) methods based on advanced MD integrators and high order factorizations of the Boltzmann operator that reduce the computational cost of path integral simulations, and their implementation in i-PI. Going beyond benchmarks, I will demonstrate their improved convergence in obtaining accurate estimates of the heat capacity of metal organic frameworks, and proton momentum distribution for various phases of water at a fraction of the computational cost that would be required if using conventional techniques.

MM 23.8   Wed 12:15   H44

Performance of van der Waals Methods at Non-Equilibrium Molecular Geometries — •Dennis Barton, Yasmine Al-Hamdani, and Alexandre Tkatchenko — Université de Luxembourg, Luxembourg, Luxembourg

An accurate description of van der Waals (vdW) dispersion interactions is a fundamental problem in electronic-structure calculations. These interactions are subtle, but of highest importance for the description of the structure, stability, and dynamics of biomolecules, chemical compounds, and materials.

Usually, approximate models for vdW interactions are used in combination with semi-local density functionals [1,2]. Common vdW methods are parametrized by one or more parameters, optimized for systems at equilibrium distances. Hence, their accuracy can only be granted at the energetic minimum.

We investigate vdW methods in terms of interatomic distances in small and weakly bound bimolecular complexes. We find a systematic increase of accuracy for the Many-Body Dispersion (MBD) method with respect to the intramolecular distance. In contrast, pairwise approaches (e.g. TS, D3) and non-local functionals show a non-systematic behavior.

Our analysis of the performance of vdW methods away from equilibrium geometries will greatly help to develop new methods with high accuracy everywhere on the potential-energy surface.

[1] Grimme *et al.*, Chem. Rev. **116**, 5105 (2016)
[2] Hermann *et al.*, Chem. Rev. **117**, 4714 (2017)

MM 23.9   Wed 12:30   H44

Limitations of the DFT–1/2 method for covalent semiconductors and transition-metal oxides — •Jan Doumont, Fabien Tran, and Peter Blaha — Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165-TC, A-1060 Vienna, Austria

The DFT–1/2 method in density functional theory [L. G. Ferreira *et al.*, Phys. Rev. B **78**, 125116 (2008)] aims to provide accurate band gaps at the computational cost of semilocal calculations. The method has shown promise in a large number of cases, however some of its limitations or ambiguities on how to apply it to covalently bonded semiconductors have been pointed out recently [K.-H. Xue *et al.*, Comput. Mater. Science **153**, 493 (2018)]. In this work, we investigate in detail some of the problems of the DFT–1/2 method with a focus on two classes of materials: covalently bonded semiconductors and transition-metal oxides. We argue for caution in the application of DFT–1/2 to these materials. Specifically, two conditions must be met for a reliable application: the electron density close to the valence band maximum must be sufficiently similar to the atomic orbital used to calculate the DFT–1/2 correction potential and the orbitals at the valence band maximum and conduction band minimum must be well separated in real space.

MM 23.10   Wed 12:45   H44

Implementation of stress tensor in LAPW method with emphasis on WIEN2k — •Kamal Belbase, Andreas Tröster, and Peter Blaha — Institute for Materials Chemistry, Vienna University of Technology, Vienna, Austria

The theoretical derivation and practical implementation of the stress tensor in all electron density functional theory (DFT) codes of the linearized augmented plane wave (LAPW) type is a long standing and demanding problem. Here we present some theoretical calculations and results for hydrostatic pressure as implemented in the WIEN2k code. Similar to the structure of force formulas, we derive the Hellmann-Feynman and Pulay contributions to the full stress tensor. Hydrostatic pressure is obtained by taking the trace of these terms. Comparison of our thereby calculated pressure to that computed from fits of the total energy using the Birch-Murnaghan's equation of state is presented for some cubic crystals.

MM 23.11   Wed 13:00   H44

Parallelization and Acceleration of the FLEUR Code: New Possibilities for All-electron Density Functional Theory — •Uliana Alekseeva, Daniel Wortmann, and Stefan Blügel — Institute for Advanced Simulation and Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The perpetual evolution of the high performance computing (HPC) hardware is a considerable challenge for scientific software, which has often been developed over decades. In particular, the need to adapt for new hardware can require substantial changes in the data layout, the parallelization strategy and the fundamental algorithms. The interplay of different functionalities amplifies the redesign challenge.

An example of such a scientific software package is the all-electron DFT code FLEUR developed at the Forschungszentrum Jülich (http://www.flapw.de). While its main field of application is the simulation of complex magnetic structures, the employed full-potential linearized augmented plane wave (FLAPW) scheme ensures a general applicability for all bulk and film setups. We will present our experiences with implementing the hybrid MPI+OpenMP parallelization, the challenges arising from finding an efficient algorithm and from optimizing the performance. In addition, we will report on porting of the code to NVIDIA GPUs. Finally, we demonstrate that the improved scalability of the code allows calculations for unit cells with over 1000 atoms.

MM 24: Topical session (Symposium MM): Correlative and in-situ Microscopy in Materials Research

Sessions: Energy Materials II; Nanomechanical Testing

Time: Wednesday 10:15–13:15   Location: H45

Topical Talk   MM 24.1   Wed 10:15   H45
Correlating electrical and mechanical behaviour of polymer supported metal thins with in-situ methods — •Megan J. Cordill — Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria

Ductile films and lines are an integral part of flexible electronics because they allow current flow between semiconducting islands and other operating features. However, the charge carrying ductile films must be of an optimum thickness and microstructure for suppression of cracking when tensile loading is applied. Studies of strained films on polymer substrates tend to emphasize only the electrical properties and thickness effects more than the role of film microstructure or deformation behavior. To address both the electro-mechanical and deformation behavior of metal films supported by polymer substrates, in-situ resistance measurements were performed with in-situ confocal scanning laser microscopy imaging of the film surface during cycling. The resistance measurements allow for the examination of the changes in resistance with strain, while the surface imaging permits the visualization of localized thinning and crack formation. Furthermore in-situ synchrotron tensile tests provide information about the stresses in the film and show the yield stress where the deformation initiates and the relaxation of the film during imaging. The combination of electrical measurements, surface imaging, and stress measurements allow for a complete picture of electro-mechanical behavior needed for the improvement and future success of flexible electronic devices.

                                          MM 24.2   Wed 10:45   H45
Correlation of conductivity and failure mechanism of silver nanowire networks: a scale bridging in situ study — •Nadine Schrenker[1], Peter Schweizer[1], Marco Moninger[1], George D. Spyropoulos[1], Mirza Mačković[1], Manuela Göbelt[2], Nikolas Karpstein[1], Silke Christiansen[2], Christoph J. Brabec[1], and Erdmann Spiecker[1] — [1]FAU Erlangen, Germany — [2]MPI, Erlangen

For flexible organic solar cells it is decisive to withstand mechanical loading without sacrificing the performance. Silver nanowire (Ag NW) networks are a highly promising electrode material, since they combine a low sheet resistance with a high transmittance, however the interplay between microscopic failure mechanisms and the functional properties of electrodes in complete OSCs has not been elucidated so far. In this work we introduce a scale-bridging in situ approach to correlate the mechanical response of Ag NW electrodes with their electrical properties starting from single wires up to complete solar cell devices. On the nanometer scale in situ STEM tensile tests of single 5-fold twinned Ag NWs reveal a localized deformation by necking and a clear size-dependence of the mechanical properties. Going up in scale, Ag NW networks on PET foils were tested by in operado SEM tensile tests. These tests show a clear dependency of the wire orientation regarding the straining direction. Buckling as well as kinking as deformation mechanism were observed for wires perpendicular to the straining direction. Moreover, the texture can be utilized to increase the conductivity at 20 % up to nine times. The phenome of kinking is analyzed via HRTEM and complementary atomistic simulation.

                                          MM 24.3   Wed 11:00   H45
In Situ and Ex Situ Electron Microscopy Studies of Al-Si Alloying at Grain Boundaries — •Christoph Flathmann[1], Hendrik Spende[2], Tobias Meyer[1], Patrick Peretzki[1], and Michael Seibt[1] — [1]4th Institute of Physics - Solids and Nanostructures, University of Goettingen, Friedrich-Hund-Platz 1, 37077 Goettingen, Germany — [2]Institute of Semiconductor Technology, Braunschweig University of Technology, Hans-Sommer-Straße 66, 38106 Braunschweig, Germany

During alloying of thin aluminium (Al) layers with bulk multicrystalline (mc) silicon (Si), Al entirely melts at temperatures above 660 °C whilst Si remains solid. Since a surplus of Si is available, the equilibrium concentration of the melt is given by the silicon-rich liquidus line at the corresponding temperature. Thus, a thermodynamic driving force for silicon dissolution is present. However, for mc Si, grain

boundaries are sites of preferred dissolution. Hence, uneven dissolution is expected in mc material.

Employing scanning electron microscopy (SEM) and electron beam induced current (EBIC), preferential dissolution, at both low symmetry grain boundaries and {111} twin boundaries, is observed for ex situ alloyed samples. Correlating SEM and EBIC signals allows for visualising the dependence of dissolution depth on electrical junction formation. Furthermore, the dynamics of preferential dissolution are studied by in situ TEM heating experiments of {111} twin boundaries.

                                          MM 24.4   Wed 11:15   H45
3D characterization of macroporous MFI-type zeolite crystals combining nano X-ray tomography and 360° electron tomography — •Dominik Drobek[1], Janis Wirth[1], Silvan Englisch[1], Tobias Weissenberger[2], Benjamin Apeleo Zubiri[1], Wilhelm Schwieger[2], and Erdmann Spiecker[1] — [1]Institute of Micro- and Nanostructure Research (IMN) & Center for Nanoanalysis and Electron Microscopy (CENEM), Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Chair of Chemical Engineering I (Reaction Engineering), Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Combining lab-based high-resolution X-ray microscopy (XRM) tomography with 360° electron tomography (ET) enables three-dimensional (3D) imaging of complex material structures across multiple length scales. MFI-type zeolite crystals, which are synthesized utilizing steam-assisted crystallization with mesoporous silica spheres as template[1], with sizes of around 3 μm featuring a well-connected intracrystalline macropore network approach the upper (XRM) and lower (ET) resolution limits of each technique. The combination of both techniques enables a complete 3D reconstruction of the pore structure enabling for quantitative analyses and, furthermore, a direct comparison of the tomography techniques themselves. For optimized imaging conditions individual particles are prepared on a tip utilizing the stamping transfer technique[2] in a dual-beam SEM/FIB instrument. References: [1] A.G. Machoke et al., Adv. Mater. 27 (6) 1066-1070, 2015. [2] T. Przybilla et al., Small Methods 2, 1700276, 2018.

15 min. break

Topical Talk   MM 24.5   Wed 11:45   H45
Pathing the way to unique, nondestructive 3D-microstructure properties by in situ Laue tomography — Jean-Baptiste Molin[1], Loïc Renversade[2,3], Jean-Sebastien Micha[2,3], and •Christoph Kirchlechner[1] — [1]Max-Planck-Institut für Eisenforschung GmbH — [2]Univ. Grenoble Alpes, CNRS, CEA, INAC-SyMMES, — [3]CRG-IF BM32, ESRF, BP 220

Interlinking the mechanical properties of materials to their underlying and evolving microstructure is vital for a mechanism-based understanding of deformation, in particular at the micron scale. Numerous characterization tools, like scanning electron microscopy (SEM), transmission electron microscopy (TEM) as well as synchrotron based Laue microdiffraction (Laue) offer a complementary toolbox being well suited to answer most questions in material science today.

However, the current toolbox is either limited to surface information (e.g. SEM), thin samples (TEM) or integrated information (Laue). To close this gap we have combined a DAXM setup with a nanoindenter at BM32 of the European Synchrotron (ESRF). The talk will primarily focus on the experimental aspects of this unique machine including its experimental limits as well as prospects of future use.

                                          MM 24.6   Wed 12:15   H45
Local Fatigue Behavior of Bimodal Copper Sheets Investigated by Dynamic Micropillar Compression — •Sebastian Krauss, Benoit Merle, and Mathias Göken — Friedrich-Alexander-Universität Erlangen-Nürnberg, Lehrstuhl Allgemeine Werkstoffeigenschaften (WW I), Erlangen, Germany

In contrast to macroscopic fatigue testing, fatigue experiments on local microsamples offer the opportunity to isolate the individual microstructural contributions from the global behavior of layered ma-

terials. In this study, Accumulative Roll Bonding (ARB) processed copper sheets with a bimodal microstructure were analyzed. Micropillars were fabricated by Focused Ion Beam (FIB) milling, yielding testing specimens positioned inside the individual layers of the material. Due to the bimodal microstructure, the microsamples from the different layers show varying grain sizes, which results in a change of the respective fatigue properties. Additionally, micropillars were prepared at the interface to study interface contributions to the fatigue behavior. The investigations were executed by a novel approach that combines dynamic nanoindentation and micropillar compression. With this technique the high cycle fatigue range is easily accessible for microscale samples. Observation of the underlying deformation processes was performed by SEM imaging as well as FIB cross-sectioning of the deformed samples.

MM 24.7   Wed 12:30   H45

Mechanical properties of nanoporous gold studied by scale-bridging in situ testing, non-destructive 3D analyses and experimentally-informed simulations — •Thomas Przybilla[1], Erich Thiess[1], Florian Niekiel[1], Benjamin Apeleo Zubiri[1], Mirza Mačković[1], Peter Schweizer[1], Zhuocheng Xie[2], Julien Guénolé[2], Arun Prakash[2], Stephen T. Kelly[3], Hrishikesh A. Bale[3], Erik Bitzek[2], and Erdmann Spiecker[1] — [1]IMN, FAU, Erlangen, Germany — [2]WW 1, FAU, Erlangen, Germany — [3]Carl Zeiss X-ray Microscopy, Pleasanton, USA

The objective of this study is to understand the interplay between the size of single struts, the network topology/morphology and the defect structure in nanoporous gold (npg). The aim is realized by combining in situ micromechanical testing with non-destructive tomographic techniques and experimentally-informed simulations. Micropillar compression is performed in scanning electron microscopy and transmission electron microscopy. For small strut sizes, 360° electron tomography is applied enabling high quality reconstructions of the npg network. The experimentally derived 3D data are used as input for large-scale atomistic simulations and compared with simulations on geometrically constructed structures. This approach allows the correlation of experimental and simulated flow stress, the explanation of defect mechanisms observed in the experiment and the study of different topology and boundary conditions. For larger strut sizes analyses are carried out by high-resolution X-ray tomography and experimentally-informed finite element simulations correspondingly.

MM 24.8   Wed 12:45   H45

Experimentally-Informed Large-Scale Atomistic Simulations of Nanoporous Gold — •Zhuocheng Xie[1], Julien Guénolé[1], Aruna Prakash[1], Thomas Przybilla[2], Erdmann Spiecker[2], and Erik Bitzek[1] — [1]Materials Science & Engineering, Institute I, Friedrich-Alexander-Universität Erlangen-Nürnberg,

Martensstraße 5, 91058 Erlangen, Germany — [2]Institute of Micro- and Nanostructure Research & Center for Nanoanalysis and Electron Microscopy (CENEM), Friedrich-Alexander-Universität Erlangen-Nürnberg, Cauerstraße 6, 91058 Erlangen, Germany

Nanoporous gold (NPG) is an ideal model system for the study of size effects at the nanoscale, since the ligament size can be precisely tailored within the nanometer to micrometer range. In this work, we study the deformation behavior of NPG using large-scale molecular dynamics simulations. We report on uniaxial compression tests using experimentally informed real-size atomistic samples, which are reconstructed from electron tomography datasets. By comparing the results of these simulations with simulations on geometrically constructed samples with average ligament size and porosity equal to the experimental samples, we study the influence of morphology and topology on the deformation behavior of NPG. The influence of surface-induced-stress on the critical resolved shear stress of NPG is evaluated by comparing the real-size samples and samples scaled-down by different factors. Additionally, the deformation mechanisms are studied in detail. The results provide qualitative insights in the fundamental deformation mechanisms not readily observable in in-situ mechanical tests.

MM 24.9   Wed 13:00   H45

Fracture toughness of predeformed chromium studied with microcantilever bending — •Stefan Gabel, Benoit Merle, Erik Bitzek, and Mathias Göken — Institute I: General Materials Properties, FAU Erlangen-Nürnberg, Germany

Cr, Mo and W are the most common bcc metals, which are characterized by a high melting point and high strength. However their fracture toughness at room temperature is low. This is due to their rather high ductile by brittle transition temperature. At room temperature the fracture toughness is limited by dislocation mobility or by the inability to activate nucleation sources. While this behavior is well researched for W, there are only few studies for Cr. FIB milled cantilevers were used to characterize the facture toughness of Cr on the microscale and to study the influence of the loading rate and the initial dislocation density of the sample. In order to achieve high dislocation densities by pre-deformation, Vickers indentations were made on the sample surface prior to testing. The resulting plastic strain field in the material was analyzed by FEM. Selecting different distances to the center of the Vickers indent allows varying the amount of pre-deformation of the cantilevers. The measurements showed that an increase of the loading rate embrittles Cr, whereas an increase of the dislocation density leads to a toughening of the sample. Furthermore the dependence of the transition in the fracture behavior on the availability dislocations and activity of dislocations sources was investigated via TEM-lamella lift-outs and Transmission Kikuchi Diffraction mapping.

MM 25: Transport (Diffusion, conductivity, heat)

Sessions: Transport I and II

Time: Wednesday 10:15–13:15   Location: H46

MM 25.1   Wed 10:15   H46

Strain induced atomic transport in ultra-fine grained Nickel — •Shraddha Sevlikar[1], Mayur Vaidya[1], Jonathan Zimmermann[2], Lishai Shoham[2], Eugen Rabkin[2], Gerhard Wilde[1], and Sergiy Divinski[1] — [1]Institute of Materials Physics, University of Muenster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Department of Materials Science and Engineering, Technion - Israel Institute of Technology, Technion City, Haifa 3200003, Israel

Strain-induced atomic transport was investigated in coarse and ultra-fine grained (UFG) Nickel using the radiotracer analysis. UFG Ni was produced by high-pressure torsion (HPT) of high purity coarse-grained Ni samples using 10 rotations and 4 GPa pressure. X-ray analysis revealed a grain size of 100 nm for the HPT sample. The radioactive isotope ^{57}Co was deposited on the sample surface with mirror-finish obtained by mechanical polishing. The HPT sample was then carefully sandwiched between tantalum foils and subjected to cold rolling to 5/20 % deformation. The tracer penetration achieved during rolling was measured by serial sectioning. A strain-induced tracer penetration was quantified and compared to thermally activated diffusion in coarse-grained and UFG Ni. Reducing the sample roughness during rolling

and limiting the extent of deformation-induced porosity are identified as major challenges in developing this experimental setup. The impact of sample microstructure on deformation-induced atomic transport is discussed.

MM 25.2   Wed 10:30   H46

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

Metal-Organic Frameworks (MOFs) represent a family of highly porous materials that have shown promising properties for numerous applications including gas-storage and catalysis. As most of the applications for MOFs rely on the effectiveness of heat dissipation, it is crucial to investigate their thermal transport properties in detail. These materials allow for easy modifications in their structural composition and architecture. Thus, an in-depth understanding of the structure-to-property

relationship will allow a precise tailoring of the material to meet individual requirements. Here we apply molecular dynamics (MD) simulations, in combination with the MOF-FF force field potential, to investigate the heat transport properties of MOFs with different composition (i.e. varying the organic and inorganic components). Special care is taken to analyze the periodic interfaces between the individual segments occurring in MOFs, as they are identified as a major limiting factor for heat transport. Furthermore, vibrational properties have been investigated in the framework of density-functional-theory, in order to provide further analysis leading to a more generally applicable prediction of the thermal conductivity for different MOF morphologies.

MM 25.3   Wed 10:45   H46

Determination of the correlation factor for Cd solute diffusion inNi_3Al — ●Bengü Tas[1], Ryan Murray[2], Gary S. Collins[2], and Sergiy V. Divinski[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Department of Physics and Astronomy,Washington State University, Pullman, WA, USA.

The correlation factor is an essential parameter for atomic transport in solids. In the case of self-diffusion, the correlation factor can be calculated easily from the lattice geometry, if the diffusion mechanism is known. Since the solute atoms modify the vacancy concentration and jump rates, measuring the solute diffusion correlation factor is a complicated task. While the first principles simulations have enabled computing the correlation factor within the framework of simplified models such as the five vacancy jump frequency model for fcc crystals, its experimental determination has never been performed. In this work, we contribute to the first measurements of the correlation factor of solute diffusion combining long-range diffusion measurements and perturbed angular correlation (PAC) experiments. The diffusion coefficient of Cd was measured at a temperature of 1073 K within the cubic $L1_2$ ordered Ni_3Al crystal structure and the impurity jump frequency was determined at the same temperature. The experimental findings are finally combined to evaluate the correlation factor of Cd atoms in the Ni_3Al sublattice.

MM 25.4   Wed 11:00   H46

Spectral and transport properties of disordered Mott systems — ●Himadri Barman — Department of Physics, Zhejiang University, 38 Zheda Road, Hangzhou, Zhejiang 230027, China — Institute of Mathematical Sciences, 4th Cross, CIT Campus, Taramani, Chennai, Tamil Nadu 600113, India

We study the disordered Hubbard model within the dynamical mean-field theory (DMFT) framework using the coherent potential approximation (CPA). Despite similar studies have been performed in the earlier literature, for the first time, we looked at the finite temperature longitudinal and transverse (Hall) conductivity and discovered two different scattering rates: one following the Fermi-liquid's quadratic temperature (T) dependence and the other showing a non-Fermi-liquid like power-law behavior. Thus our theoretical results show that the interplay of disorder and Coulomb interaction may possess the answers to the long-standing unresolved problem of the two-scattering rates discovered in the cuprates, and subsequently in the bulk correlated oxide materials.

MM 25.5   Wed 11:15   H46

Low-energy electron attachment induced transport - conductivities and the role of blocking electrodes — Anneli Hein, Martin Schäfer, and ●Karl-Michael Weitzel — Philipps-Universität Marburg, Fachbereich Chemie

The charge carrier transport in an alkali ion conducting glass has been investigated by means of the charge attachment induced transport (CAIT) technique [1]. For the first time we describe the direct measurement of the absolute bulk conductivity and the activation energy for ion hopping in a glass by attachment of low-energy electrons to the front side of a glass, which is in contact with a single metal electrode at the backside [2]. The electron attachment experiment induces electro-diffusion of mobile cations towards the front side of the sample. In the limit of short time respectively little charge transported this approach allows measuring the conductivity as well as the activation energy of the glass, which agree well with reference measurements. In the limit of long time respectively considerable charge transported alkali depletion profiles evolve at the interface between the electrode and the glass. This eventually gives rise to the blocking of charge transport. A quantitative model for the evolution of "blocking electrode" characteristics is presented. The mechanism involves transient dielectric breakdown. [1] J. Martin, M. Gräf, T. Kramer, C. Jooss, M.J. Choe, K. Thornton,

K.-M. Weitzel, PCCP, 19, 962, (2017) [2] A. Hein, M. Schäfer, K.-M. Weitzel, in preparation

15 min. break

MM 25.6   Wed 11:45   H46

Bulk diffusion of Mn in α-iron — ●Vladislav Kulitckii, Sergiy Divinski, and Gerhard Wilde — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Münster, Germany

The impact of a magnetic transition on bulk diffusion of Mn in α-iron is studied by microtome (higher temperatures) - and ion-beam sputtering (low temperatures) - sectioning using the radioactive isotope 54Mn. The experiments were performed in the temperature range of 773 to 1173 K. In contrast to the case of self-diffusion [1, 2], a marginal * if any * impact of the magnetic transition in α-Fe on Mn bulk diffusion is observed with almost the same linear Arrhenius dependences below and above the Curie temperature. No distinct deviation from a linear Arrhenius temperature dependence is observed and the Mn bulk diffusion coefficient can be given by the pre-exponential factor D0 = 2.87*10-2 m2/s and the activation enthalpy Q = 282.8* 6.7 kJ/mol in the whole temperature interval under investigation. [1] Y.Iijima, K.Kimura, K.Hirano. Acta Metall. 36 (1988) 2811-2820. [2] M.Lübbehusen, H.Mehrer. Acta Metall. 38 (1990) 283-292

MM 25.7   Wed 12:00   H46

Impact of paramagnetic excitations and relaxations on diffusion in Fe-Mn alloys — ●Omkar Hegde, Osamu Waseda, Tilmann Hickel, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Understanding the impact of paramagnetism on defect kinetics is, though conceptually and computationally challenging, important for designing Fe-based alloys. Since magnetic degrees of freedom change faster than atomic degrees of freedom in the paramagnetic state, the atoms move according to an averaged force instead of instantaneous forces attained from each spin configuration. Therefore, a new computationally efficient method based on spin-space averaging (SSA) has been developed to handle magnetic disorder next to defects. The method uses the spin constraint tool developed and implemented in the DFT code S/PHI/nX. The performance of the method is demonstrated for local atomic relaxations next to point defects. For α-Fe, we show that both magnetic disorder and local relaxations significantly affect vacancy formation and migration energies. Next, we focus on the FeMn system, for which the vacancy formation energy as a function of Mn concentration for both ferromagnetic and paramagnetic cases is presented. We demonstrate that paramagnetism significantly affects atomic relaxations as well as diffusion barriers and thereby explain why Mn diffusion shows a different temperature dependence than Fe-self diffusion in α-Fe.

MM 25.8   Wed 12:15   H46

On Stochastic Resonance in Double Resonance Models — ●Amit Chattopadhyay[1] and Elias Aifantis[2] — [1]Systems Analytics Research Institute, Mathematics, Aston University, Birmingham, UK — [2]Laboratory of Mechanics and Materials, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece

Double diffusion as a model of transport involving two interacting species is essentially a continuum model with two local non-equilibrium concentration fields obeying separate mass and momentum balance equations, with a linear relation for the mass exchange term between them. Here we present results from two separate stochastic double-diffusion models involving two fluctuating phase densities, which represent the same system for two different symmetry cases. We show that presence of surface inhomogeneities and temporal delay have substantial impact at the interface of evolution for both models. The effect is most pronounced at a critical point, identified as the "stochastic resonance" [1,2] point where maximum energy transfer occurs that create complementary profiles for the spatial and temporal correlation functions. The symmetry difference between the two models lead to spatiotemporal patterns that are unique to each individual case. Model results verify a multitude of interface based experiments concerning nanomaterial dynamics.

References: [1] AKC & ECA; Physical Review E, vol 95, 052134 (2017). [2] AKC, et al;, Materials Science and Technology, vol 34:13, 1606 (2018).

MM 25.9   Wed 12:30   H46

Low-temperature heat capacity of Fe-Mn alloys — •Marius Gerlitz, Martin Peterlechner, Sergiy Divinski, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Germany

For a fundamental description of ferromagnetic materials, knowledge of characteristic thermodynamic properties is essential. The analysis of the magnetocaloric effect or magnetostriction is a significant step, feasible by specific heat measurements. The influence of magnetism, chemical composition and short-range order on the specific heat capacity of a series of Fe-Mn alloys (up to 9.5 at.% Mn) is systematically measured in the temperature interval between 1.9 K and 400 K. A physical properties measurement system (PPMS) is used and the 2-tau method is applied for the analysis. Additionally, a constant magnetic field of 3 T is applied to determine the impact of an external field. Furthermore, calorimetric measurements by differential scanning calorimetry (DSC) are performed using heating rates of 20 K/min in the temperature interval from 300 K to 723 K. Thermal - and magnetic entropy contributions are determined. The Debye temperatures and the electronic contribution to the specific heat are estimated. The results are discussed with respect to the chemical composition and probable short-range ordering.

MM 25.10   Wed 12:45   H46
Thermal properties of solids determined by lock-in infrared thermography — •Nils Ziegeler[1], Peter W. Nolte[2], A. Charlotte Rimbach[1], and Stefan Schweizer[1,2] — [1]South Westphalia University of Applied Sciences, Lübecker Ring 2, 59494 Soest — [2]Fraunhofer Application Center for Inorganic Phosphors, Branch Lab of Fraunhofer Institute for Microstructure of Materials and Systems IMWS, Lübecker Ring 2, 59494 Soest

As material science advances and more and more materials are developed, their use cases become increasingly specialized. In thermal design, a precise knowledge of the thermal parameters, such as the thermal diffusivity and the thermal conductivity, has to quickly be at hand if required.

Here, contactless lock-in infrared thermography is used to determine the thermal diffusivity value of a material. The method consists of a point-like heat source (such as a laser), which periodically heats the front side of the sample. The generated heat waves travel though the specimen and are detected on the backside by an infrared camera. In lock-in thermography, the phase delay between the periodic heating on the front and the temperature variations on the rear side is analyzed. Since the phase delay depends on the modulation frequency, a series of measurements is performed to determine the thermal diffusivity of the material. The principle is demonstrated on lithium borate glass of varying composition. The results show that even small changes in chemical composition can be detected.

MM 25.11   Wed 13:00   H46
Investigations of ionic transport in bicrystals of Sr-doped LaMnO$_3$ — •Jacqueline Marie Börgers[1,2] and Roger De Souza[1] — [1]Institute of Physical Chemistry, RWTH Aachen University, Aachen, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, Jülich, Germany

Mixed-valence manganites are very promising candidates as materials for resistive switching due to the possibility to generate multilevel resistance states as well as area-dependent switching. This enables their use in future non-volatile memory or novel neuromorphic circuits.

It is widely accepted that ionic transport plays an important role in the field of resistive switching. Also for manganites the key mechanism is assumed to be drift and diffusion of oxygen vacancies. Additionally, by varying the composition and microstructure of manganites the electronic and ionic transport properties can be influenced. The aim of this study is to illuminate the relationship between structural factors of the material and its switching performance. Hereby, we are particularly interested in the influence of grain boundaries on the transport mechanisms.

Therefore, the ionic transport along grain-boundaries in Sr doped LaMnO$_3$ ((La$_{1-x}$Sr$_x$)MnO$_{3\pm\delta}$,LSMO) is studied in order to gain further insight on its switching mechanisms. The migration of oxygen ions in bicrystals of LSMO is studied by Molecular Dynamics (MD) simulations employing empirical pair potentials. In addition, static atomistic simulations are used to gain further insights into defect formation processes.

MM 26: Materials for Energy Storage and Conversion

Sessions: Li-Batteries and Alternative Concepts

Time: Wednesday 15:00–18:15   Location: H43

MM 26.1   Wed 15:00   H43
Studying the cycling behavior of Silicon thin-film battery electrodes by in-situ quartz crystal microbalance — •Tobias Kohler, Efi Hadjixenophontos, and Guido Schmitz — Chair of Material Physics, Institute of Materials Science, University of Stuttgart, Heisenbergstraße 3, 70569 Stuttgart, Germany

A quartz crystal microbalance (QCM) is able to detect mass changes in the nanogramm region. This makes it suitable to monitor the lithiation and delithiation of battery electrodes. Some particle-binder composite electrodes were already researched by means of QCM. However, investigations of thin-films are scarce. Here, amorphous silicon electrodes were ion beam sputter deposited onto the front electrode of the quartz crystal. By combining the QCM results with the cyclic voltammetry (CV), a variety of information can be gained. This includes a mass per charge ratio, which is similar to a conventional mass spectrometry. It opens the possibility to measure the growth of the solid electrolyte interface (SEI) and determine the species that are included therein. Different thicknesses of silicon are investigated to see the effect on the SEI layer growth. The results of the QCM are compared to electron microscopy and X-ray photoelectron emission spectra observations.

MM 26.2   Wed 15:15   H43
Electrochromism and Phase Transformation in Lithium Titanate — •Yug Joshi, Efi Hadjixenophontos, and Guido Schmitz — Chair of Materials Physics, Institute of Material Science, University of Stuttgart, Stuttgart, Germany

Lithium titanate (LTO) is a well-known battery anode mainly due to its high rate capability, high cyclability and high power density. In the potential range between 1V-2V vs Li/Li+, intercalation appears between two phases i.e. Li7Ti5O12 (stable below ca. 1.55V) and Li4Ti5O12 (stable above ca. 1.55V). While there is negligible volumetric change, the two phases show contrasting dielectric constants and complex refractive indices. Our study is based on understanding the phase transformation mechanism of LTO by exploiting these contrasting properties in the two phases. To realize this, firstly the active LTO layer is deposited using ion beam sputtering and annealed appropriately. The crystal structure of the layers are probed using X-ray diffraction and transmission electron microscopy. Once the crystal structure is confirmed, the samples are electrochemically characterized. Finally, the electrochromic characterization is performed in-situ and ex-situ to visualize the electrochromic reversibility and to extract the complex refractive indices. The latter are used to calculate the dielectric constants in the single- and in the dual-phase regions. Describing the dielectric constant of the dual phase region as a combination of those of the pure phases, information is derived about the migration of the phase front during transformation.

MM 26.3   Wed 15:30   H43
Electrochemical and Microstructural Analysis of High-capacity Li-Mn-O Thin Film Battery Electrodes — •Henry Müller, Yug Joshi, Efi Hadjixenophontos, Claudia Peter, and Guido Schmitz — Institute of Materials Science, Chair for Materials Physics, University of Stuttgart, Heisenbergstraße 3, 70569 Stuttgart, Germany

Research worldwide has taken on the challenge to develop new electrode materials for cost-efficient, reliable batteries with higher capacities. We present a sputter-deposited thin film cathode made from manganese oxide with up to three times the capacity observed in comparable conventional LiMnO electrodes from the well-known spinel structure. The novel microstructure, domains of rock salt, monoclinic and spinel crystal structures, unlocks the voltage range from 2V to 4.4V vs.

Li for long term cycling at the capacity of 225 mAh/g. We characterize the material on the nano-scale using high-resolution transmission electron microscopy and electron diffraction. Furthermore, we investigate the influence of oxygen deficiency on the capacity and electrochemical behavior of the electrode. The in-situ tailoring of electrode properties is possible by controlling the oxygen partial pressure during deposition.

MM 26.4   Wed 15:45   H43
Analytical Transmission Electron Microscopy studies of $LiNi_xMn_yCo_{1-x-y}O_2$ and Silicon electrode materials for lithium ion batteries — •Ardavan Makvandi[1], Martin Peterlechner[1], Simone Casino[2], Tobias Gallasch[2], Martin Winter[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]MEET Battery Research Center, University of Münster, Münster, Germany

The modification of state-of-the-art electrode materials by nanostructured coatings is one approach to optimize crucial parameters for application, such as electronic conductivity or mechanical stability of the raw materials. In general, interfaces (active material/coating; electrode surface/electrolyte) determine the local Li ion transport kinetics and finally the electrochemical cell performance in terms of cycling stability or capacity retention. Therefore, it is necessary to study the structure and chemistry of electrodes and electrode/electrolyte interfaces. In this work, the structural and chemical evolution in the bulk and surface regions of $LiNi_xMn_yCo_{1-x-y}O_2$ (NMC) and silicon thin film electrodes after lithiation and de-lithiation processes is studied using scanning transmission electron microscopy (STEM) imaging, electron diffraction, and electron energy loss spectroscopy (EELS). In case of EELS quantification, the Mn-M edge overlaps with the Li-K signal hindering the direct measurement of the lithium content. Nonetheless, by using EELS, the valence states of transition metals (Mn, Co, and Ni) and consequently an indirect measurement of the lithium ion distribution in the NMC cathode materials can be obtained.

MM 26.5   Wed 16:00   H43
Investigation of micro batteries containing single secondary particles of $Li(Ni_{1-x-y}Co_xMn_y)O_2$ as cathode material — •Markus Sebastian Friedrich[1,2], Simon Burkhardt[1,2], Matthias Thomas Elm[1,2,3], and Peter Jens Klar[1,2] — [1]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Center for Materials Research (LaMa/ZfM), Heinrich-Buff-Ring 16, 35392 Giessen — [3]Institute of Physical Chemistry, Heinrich-Buff-Ring 17, 35392 Giessen

Lithium ion batteries (LIBs) are todays state-of-the-art power supplies for portable electronic devices as well as for electrical and hybrid vehicles. To optimize such battery systems, a deeper understanding of the transport in the active material used in the electrodes of LIBs is essential. Typically layered structured transition metal oxides, such as $Li(Ni_{1-x-y}Co_xMn_y)O_2$ (NCM), are used as cathode active materials. Conventionally, for investigation, micrometer sized secondary particles of the active material, built from a complex porous network of nanometer sized single crystalline primary particles, are incorporated in to composite electrodes, which contain additives that might influence or superpose the properties of the pure active material.

We developed a technique to assemble micro batteries that contain single secondary particles of NCM and performed electrochemical measurements on such cell systems. In the course of these investigations, we found clear evidence that the transport in the active material particles depends on the secondary particle diameter and, therefore, depends on the porous primary particle network.

MM 26.6   Wed 16:15   H43
poly(10-(4-styrene)-N-10H-phenothiazine) (PS-N-PT) as organic redox-active cathode materials for lithium-ion batteries — •Yuquan Wu[1], Fabian Otteny[2], Birgit Esser[2], and Rüdiger Klingeler[1] — [1]Kirchhoff-Institute for Physics, Heidelberg University, 69120 Heidelberg, Germany — [2]Institut für Organische Chemie, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg, Germany

Organic redox-active materials provide an environmentally friendly alternative to traditional inorganic electrode materials for lithium ion batteries. Due to structural stability and high-cycling performance, redox-active organic polymers are competitive candidates in this respect. We report electrochemical studies on the redox-active polymer poly(10-(4-styrene)-N-10H-phenothiazine) which is investigated with respect to its feasibility as cathode material. Cyclic voltammetry shows two pairs of redox peaks centered at 3.6 and 4.2 V, respectively, with a separation of 0.05 V. Changes of redox behavior between 1st and

2nd cycle indicate conformational changes on the polymer structure upon the first cycle at high voltage range of 4 - 4.5 V which cause electrochemical activation of the material. Galvanostatic cycling of the activated material between 3 and 4 V shows capacity amounts to 72 mAhg-1 in cycle 2 and capacity retention of 85% by cycle 100.

15 min. break

MM 26.7   Wed 16:45   H43
Investigation of the stoichiometry of $Ce_{1-x-y}Pr_xZr_yO_{2-\delta}$ single crystals — •Jurek Lange[1], Kathrin Michel[2], Gregor Ulbrich[3], Marbin Lerch[3], Sangam Chatterjee[1], Matthias Elm[1], and Detlev Hofmann[1] — [1]Institute of Experimental Physics I and Center for Materials Research, Heinrich-Buff-Ring 16, Justus-Liebig-University Giessen, D-35392 Giessen, Germany — [2]Institute of Physical Chemistry, Heinrich-Buff-Ring 17, Justus-Liebig-University Giessen, D-35392 Giessen, Germany — [3]Institute of Chemistry, Technical University Berlin, Strasse des 17. Juni 135, D-10623 Berlin, Germnay

The solid solution of ceria and praseodymia is interesting, as oxygen storage capacity and electrical conductivity are enhanced at the intermediate temperature range. Thus, we investigated single crystals of $Ce_{1-x-y}Pr_xZr_yO_{2-\delta}$ grown by the skull melting technique and powders of the binary compounds $CeO_{2-\delta}$ and $Pr_6O_{11-\delta}$ by electron paramagnetic resonance (EPR) and photo-EPR experiments. The methods are able to identify and to determine the energy positions of recharging levels in respect to the valence and conduction band of the material. In the as prepared samples we observe the characteristic spectrum of Pr^{4+} caused by the interaction of the unpaired 4f electron and the nuclear spin of $I = 5/2$ (abundance 100 %). We followed the evolution of the spectra upon annealing which effects the oxygen in the material.

MM 26.8   Wed 17:00   H43
Rational surface engineering toward optimizing hydrogen evolution activity of nanoporous electrodes — •Long Liu, Huaping Zhao, Yang Xu, Chenglin Zhang, Yaoguo Fang, and Yong Lei — Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany

A rational surface engineering strategy for nanoporous electrodes is demonstrated to promote the hydrogen evolution (HER) process. Cobalt nanopore arrays (CoNPA) were fabricated as a reprenentive HER electrode and subsequently functionalized by a conformal ultrathin titanium dioxide (TiO2) with optimized thickness and thereafter a well-dispersed platinum (Pt) nanoparticles with an ultralow mass loading (ca. 54 μg cm-2) anchored on TiO2 layer. The advanced features of nanoporous architecture, the improved wettability by TiO2 layer, and the abundant reactive sites arising from well-dispersed Pt nanoparticles synergistically contribute to enhance the HER kinetics of CoNPA electrodes in alkaline conditions, and finally achieved low overpotential of 29 mV, small Tafel slope of 42 mV per decade as well as long-termed performance and structure stability. Not limited to the HER electrodes, the similar strategy is also expected to be further applied to design nanoelectrodes for other electrochemical energy conversion and storage devices.

MM 26.9   Wed 17:15   H43
On the proper characterization of OER catalysts: The role of experimental and preparation parameters — •Sabita Bhandari[1], Praveen Narangoda[1], Marc Tesch[1], Ioannis Spanos[1], Robert Schlögl[1,2], and Anna Mechler[1] — [1]Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr — [2]Fritz Haber Institute of the Max Planck Society, Berlin

For kinetically slow oxygen evolution reaction (OER), the use of a catalyst is essential to make it energetically efficient and many research works on finding a novel catalyst are ongoing. Nowadays, operando studies - utilizing various techniques - are carried out to obtain a fundamental understanding of the intrinsic catalytic properties. However, how a catalyst performs under an oxidative condition of OER is determined not only by its intrinsic catalytic property but also by some experimental parameters. Generally for a powdered sample, catalyst ink is made with a suitable binder and deposited as thin layers on electrode substrate and subsequently, the electrochemical analysis is carried out in an electrolyte solution of choice. So, factors such as the electrode substrate, binder, electrolyte impurities, pH and concentration, type of gas saturated in electrolyte etc. might affect the overall performance of a catalyst. These parameters are important as these can affect the

true active species formed during electrocatalysis.[1],[2] In this study, we give an overview of the influence of some of the above-mentioned factors on the catalytic performance of a commercially available NiCo oxide for OER. [1] J. Electrochem. Soc., 2015, 162(10), F1144-F1158. [2] J. Electrochem. Soc., 2015, 162(12), F1384-F1396.

MM 26.10 Wed 17:30 H43
Photo-electrochemical properties of GaNP epitaxial films grown by MOCVD — ●René Couturier[1], Peter Ludewig[2], Wolfgang Stolz[2,3], Kerstin Volz[3], Sangam Chatterjee[1], and Detlev M. Hofmann[1] — [1]Institute of Experimental Physics I, Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, D-35392 Gießen, Germany — [2]NAsPIII/V GmbH, Am Knechtsacker 19, D-35041 Marburg, Germany — [3]Faculty of Physics and Materials Sciences Centre, Philipps-Universität Marburg, Hans-Meerwein-Str. D-35032 Marburg, Germany

Efficient charge transfer at the semiconductor-electrolyte-interface is very crucial for photo-electrochemical applications like water splitting. A very promising material for such electrochemical applications are $Ga_{1-x}N_xP$ semiconductor films. The films show charge-carrier injection under irradiation into the electrolyte, depending on the applied bias. Electron- and hole-transfers are achieved. The processes are investigated by wavelength dependent photocurrent measurements under applied potentials. In parallel, the emission properties of the material are investigated which dominantly show the recombination via clusters of nitrogen dopants. The results are discussed in the frame of the surface band-bending model.

MM 26.11 Wed 17:45 H43
A gasochromic Back Reflector for a Switchable Ultra-Thin Germanium Solar Cell — ●Maximilian Götz, Maren Lengert, Norbert Osterthun, Kai Gehrke, Martin Vehse, and Carsten Agert — DLR-Institut für Vernetzte Energiesysteme e.V. Carl-von-Ossietzky-Str. 15 26129 Oldenburg

Magnesium-Palladium (Mg/Pd) layers are gasochromic materials, which undergo a reversible phase change from a metallic-reflective into a dielectric-transparent state upon hydrogen exposure.

In this contribution we present this layer stack as a switchable mirror for use in a Fabry-Pérot absorber. This is used to modify an ultra-thin amorphous Germanium solar cell into a switchable photovoltaic device. Germanium is placed between a transparent conductive oxide and the gasochromic switchable layer, which is used as a back reflector. Due to Hydrogen exposure the cavity resonance is decreased to single pass absorption and the layer stack becomes transparent.

Optical and material properties of the cavity are characterized by in-situ spectroscopy and ellipsometry during the switching process. Optical simulations are used to adjust the thicknesses and refractive indices of the resonator materials for optimized field enhancement in the Germanium absorber. The electrical properties of Mg/Pd as back-contact for solar cell applications are discussed and the diode behavior of the cell under illumination in reflective and transparent state is shown.

MM 26.12 Wed 18:00 H43
Experimental study on the electronic structure of ZrNiSn half-Heusler thermoelectric material — ●Chenguang Fu[1], Mengyu Yao[1], L. Z. Maulana[2], Gudrun Auffermann[1], Gerhard Fecher[1], M. Dressel[2], A. V. Pronin[2], and Claudia Felser[1] — [1]Max Planck Institut für Chemische Physik Fester Stoffe, 01187 Dresden, Germany — [2]Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany

ZrNiSn-based half-Heusler compounds have been developed as good thermoelectric materials in the past decades, which are believed to be attributed to their excellent electrical power factor. However, there is still very few direct experimental investigation of the intrinsic electronic structure for this system, which actually is significant to understand the origin of their excellent thermoelectric properties. In this work, we have successfully grown high-quality undoped and doped ZrNiSn single crystals. With these crystals, we were able to measure their optical reflectivity in the frequency range from 80 cm-1 to 18000 cm-1 and to perform a systematic high-resolution ARPES study on their intrinsic electronic structure. It is found that the band gap of ZrNiSn single crystals is about 0.5 ~ 0.6 eV, which is in agreement with the DFT calculations result, but much larger than the value of 0.2 ~ 0.3 eV previously reported in polycrystalline samples. The possible reasons for this difference will be discussed.

MM 27: Methods in Computational Materials Modelling (methodological aspects, numerics)

Sessions: Alloys and Mechanical Response

Time: Wednesday 15:00–18:15   Location: H44

MM 27.1 Wed 15:00 H44
Phase stability and disorder in ThMn12 type ferromagnetic intermetallics — ●Anna J. Lehner[1,2], Daniel F. Urban[2], and Christian Elsässer[2] — [1]IAM-CMS, KIT, Karlsruhe, Germany — [2]Fraunhofer IWM, Freiburg, Germany

Rare earth (RE) and transition metal (TM) intermetallics of the ThMn$_{12}$-structure type ('1-12') are widely discussed as good candidates in the search for new hard magnetic materials with considerably less RE-content than state-of-the-art $Nd_2Fe_{14}B$ or $SmCo_5$ magnets. Some binary RE-Fe phases with ThMn$_{12}$ structure, namely the most promising NdFe$_{12}$, are experimentally stable only as thin films. By addition of alloying elements (e.g. Ti) stable ternary bulk crystals with the ThMn$_{12}$ structure can be obtained experimentally and serve for validation of promising intrinsic magnetic properties which have been predicted by a screening using density functional theory [1]. In addition to magnetic properties, predicting thermodynamic phase stabilities extends the value of the computational screening. In this study we focus on the effects of configurational disorder on the thermodynamic phase stability. We combine combinatorial first-principles total energy calculations with a cluster expansion (CE) for the configurational energy associated with TM site disorder. We relate the basis functions of the CE to the structural motifs in the topologically closed packed (tcp) 1-12 phase and discuss the transferability of our model to other tcp phases. Finally, the robustness of the CE-model for substituents of varying atomic radius (Co,Si,Ti) is critically assessed. [1] W. Körner, G. Krugel, and C. Elsässer, Sci. Rep. 6, 24686 (2016).

MM 27.2 Wed 15:15 H44
Ab initio study of plastic deformation in Fe$_2$Nb Laves phase — ●Alvin Noe Ladines[1], Thomas Hammerschmidt[1], Ali Zendegani[2], Tilmann Hickel[2], Ralf Drautz[1], and Joerg Neugebauer[2] — [1]ICAMS, Ruhr-Universität Bochum, Germany — [2]Max Planck Institute for Iron Research, Düsseldorf, Germany

The Fe$_2$Nb Laves phase is technologically relevant for strengthening advanced stainless steels. An atomistic understanding of the mechanisms of plastic deformation of this phase is lacking. We use density functional theory (DFT) to calculate the generalized stacking faults for various deformation modes. Our calculations reveal that synchroshear is the most energetically favorable deformation mechanism for the C14-Fe$_2$Nb Laves phase. We further study the influence of intrinsic point defects and alloying elements Al, Si, Cr, Ni, Mo and Zr on the energy of the stacking faults. Vacancies tend to lower the energy barrier for synchroshear deformation, while anti-site defects do not have a systematic effect on stacking fault energies. The alloying elements are shown to soften the C14-Fe$_2$Nb Laves phase.

MM 27.3 Wed 15:30 H44
Understanding the thermodynamics and kinetics of precipitate formation in Al-Sc-Zr alloys — ●Ankit Gupta[1], Yulia Buranova[2], Vladislav Kulitcki[2], K. Li[3], Yong Du[3], Biswanath Dutta[1], Tilmann Hickel[1], Jörg Neugebauer[1], Gerhard Wilde[2], and Sergiy V. Divinski[2] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]Institute of Materials Physics, University of Münster, Germany — [3]Institute for Materials Microstructure, Central South University, Changsha, China

The thermal stability of Al-based alloys is enhanced typically by improving the coarsening resistance of second phase particles. A classic example is the addition of Zr to Al-Sc alloys where the Zr segregation at particle-matrix interfaces thermally stabilizes the Al$_3$Sc particles. Our

experiments performed under varying processing conditions result in a rich microstructure characterized predominantly by two types of second phase $Al_3(Sc,Zr)$ particles: one with uniform distribution of Sc and Zr and the other with a Sc-rich core and Zr-rich shell. The chemically heterogeneous core-shell structure exhibits an anisotropic Zr distribution along different orientations of precipitate interfaces. Using DFT based calculations, we quantify this sensitive interplay between the bulk and interfacial thermodynamics causing the observed two-phase microstructure. The computed mixing enthalpy trends predict homogeneously distributed Sc and Zr on the Sc-sublattice to be the thermodynamically stable configuration. The relevance of interfacial segregation and solute interactions in explaining the chemical anisotropy and the subsequent growth of core-shell structures are shown.

MM 27.4   Wed 15:45   H44

Multi-Scale Modelling of Guinier-Preston Zone Formation in Al-Cu Alloys — •Tobias Stegmüller and Ferdinand Haider — University of Augsburg, Institute for Physics, Chair for Experimental Physics I, 86135 Augsburg, Germany

The investigation of precipitation processes in modern aluminium alloys plays an important role for the design of many material properties like strength or corrosion resistance. The influence of ageing time and temperature constitute the key for a quantitative understanding of precipitate formation.

The prediction of the evolution of the precipitate size distribution is a powerful tool for the characterisation of an alloy temper state. In this work a multi-scale approach, covering nucleation, growth and coarsening of early stage precipitates in binary Al-Cu alloys, the Guinier-Preston zones (GPZ), will be presented. Starting from DFT calculations and Cluster Expansion construction, followed by Monte Carlo free energy calculations, a meso-scale Cluster Dynamics model is constructed. By following this approach, the model is able to predict the evolution of size distributions of GPZ for different alloy compositions and ageing temperatures.

To validate the model, kinetic Monte Carlo simulations on the precipitation of GPZ were performed and the results for the evolution of average precipitate size, precipitated fraction of solute and the number density of precipitates agree well with the results obtained by Cluster Dynamics. The formulation of the multi-scale approach, its results and the comparison to the Monte Carlo simulations will be presented.

MM 27.5   Wed 16:00   H44

mergence of complex patterns in $CoTi_xZr_{1-x}Sb_{1-y}Sn_y$ and $NiTi_xZr_{1-x}Sb_{1-y}Sn_y$ half-Heuslers — •Joaquin Miranda Mena and Thomas Gruhn — Biomaterials, Universität Bayreuth, Universitätsstraße 30, D-95447 Bayreuth, Germany

We present the effects of the chemical substitution on the phase separation of alloyed half-Heuslers with formula $CoTi_xZr_{1-x}Sb_1 - ySn_y$ and $NiTi_xZr_{1-x}Sb_{1-y}Sn_y$ over a wide range of x and y concentrations. The combination of different length-scales methods -Density Functional Theory, Monte Carlo simulations and Mean field calculations- allows us to predict macroscopic properties which are relevant for the material production. We found that complex textures composed of different phases emerge for certain concentrations as the temperature is lowering. These textures could open a new strategy to reduce the heat conductivity which is hampering the performance of half-Heuslers as good thermoelectrics.

MM 27.6   Wed 16:15   H44

First principle studies of Electronic, Magnetic, and mechanical properties of (Pt and Ru) ZrTiAl Quaternary Heusler Alloy — •Ramesh Paudel[1] and Jingchuan Zhu[1,2] — [1]School of Materials Science and Engineering, Harbin Institute of Technology, Harbin 150001, China — [2]2.*National Key Laboratory of Science and Technology on Advanced in Special Environments, Harbin Institute of Technology, Harbin 150001, China

In this study, we investigated the structural, magnetic, mechanical properties of (Pt and Ru) ZrTiAl quaternary Heusler alloys by utilizing density functional theory within the CASTEP code. Investigated equilibrium lattice parameters of these compounds are in great concurrence with other theoretical work. The total magnetic moments of (PT and Ru) ZrTiAl were obtained to be 3*B and 2.99*B per unit formula respectively obeys the Slater Pauling rule. (PT and Ru) ZrTiAl is found to have a spin-flip/half-metallic gap in the minority spin channel while the majority spin channel is metallic. Therefore, both composites showed half-metallic nature and 100 percent spin polarization at the Fermi level. The calculated mechanical results revealed that both

materials are mechanically steady and ductile nature. The RuZrTiAl alloy is predicted for the very first time by utilizing the GGA scheme. Our investigated results could be worthwhile for future experimental work and application for spintronic devices.

15 min. break

MM 27.7   Wed 16:45   H44

Numerical simulation of deformation of aluminum alloy during novel Conform-HPTE process — •Jiamin Hu[1,2], Roman Kulagin[2], Yulia Ivanisenko[2], and Hui Zhang[1] — [1]College of Materials Science and Engineering, Hunan University, Changsha 410082, China — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe 76021, Germany

In this paper, we explored the feasibility of a new continuous severe plastic deformation (SPD) technique, which combines continuous extrusion forming (Conform) and high pressure torsion extrusion (HPTE), we defined it as Conform-HPTE. A finite element method (FEM) simulation model of this process was established using QForm software. The results showed that the novel Conform-HPTE technique can owe both the advantages of Conform and HPTE, thus it could be used for industrial production of aluminum alloys due to its low energy input, no limit for billet length and large shear strain during one deformation pass. The effects of tool geometry and processing parameters on the extrusion load, temperature, strain evolution and metal flow during the Conform-HPTE process were discussed.

MM 27.8   Wed 17:00   H44

Hydrogen enhanced cross-slip of dislocations in the vicinity of grain boundaries in nickel — •Ali Tehranchi, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

Extensive experimental observations indicate the presence of nanovoids and an increase of the free volume along grain boundaries in hydrogen contaminated metals. This phenomenon is rate-dependent and assumed to be connected to hydrogen embrittlement of Ni based alloys. However, an understanding of the underlying mechanism is lacking. In the present study a mechanism for an enhanced cross slip of the dislocations in the close vicinity of the grain boundaries is demonstrated by performing molecular dynamics (MD) simulations. The interaction of the screw dislocations with a variety of symmetric tilt grain boundaries in H-charged and H-free bicrystalline nickel specimens are examined. The presence of the segregated hydrogen atoms at the grain boundaries induces a stress field around them and thus the barrier for cross-slip of screw dislocations considerably decreases. The enhanced cross slip of dislocations facilitates the formation of jogs *below a critical loading rate *. These jogs are found to emit vacancies during glide processes. The mechanism discovered in this study shows nano-scale evidence of a rate sensitive enhanced vacancy formation and a subsequent increase in the free volume along the grain boundaries in the presence of H.

MM 27.9   Wed 17:15   H44

Electronic structure and lithium storage mechanism of high-rate niobium oxide-based crystallographic shear phases from first principles — •Can P. Koçer[1], Kent J. Griffith[2,3], Clare P. Grey[3], and Andrew J. Morris[4] — [1]Theory of Condensed Matter, Cavendish Laboratory, University of Cambridge — [2]Department of Materials Science and Engineering, Northwestern University — [3]Department of Chemistry, University of Cambridge — [4]School of Metallurgy and Materials, University of Birmingham

Crystallographic shear phases of niobium oxide have shown unprecedented high-rate performance as high-voltage anodes for lithium ion batteries [1,2]. The electronic structure, lithium insertion mechanism, and lithium dynamics of these compounds remain relatively unexplored, largely due to their novelty and complexity. In this talk, I will present recent work by our group on the electronic structure and lithium insertion mechanism of crystallographic shear phases in the Wadsley-Roth family, including mixed-metal TiO_2-Nb_2O_5, and WO_3-Nb_2O_5 phases. Our work has explored interesting electron localisation-delocalisation transitions on n-type doping in the niobium suboxides [3], and provides a unified mechanistic picture for the structural changes in the entire family of crystallographic shear phases [4]. I will discuss challenges associated with modelling these materials, and will point out future directions for experimental and first-principles studies.

[1] K. J. Griffith et al., Nature **559**, 556-563 (2018) [2] K. J. Griffith et al., Journal of the American Chemical Society **138**, 8888 (2016) [3]

C. P. Koçer et al. (*in preparation*) [4] C. P. Koçer et al. (*in preparation*)

MM 27.10　Wed 17:30　H44

Effect of strain on ionic conductivity of cubic Li6.25Al0.25La3Zr2O12 solid electrolyte — •Ashkan Moradabadi[1,2] and Payam Kaghazchi[3] — [1]Physikalische und Theoretische Chemie, Institut für Chemie und Biochemie, Freie Universität Berlin Takustr. 3, 14195, Berlin — [2]FG Materialmodellierung, Technische Universität Darmstadt, Otto-Berndt-Str. 3 64287 Darmstadt — [3]Forschungszentrum Jülich GmbH, Institute of Energy and Climate Research, IEK-1, D-52425 Jülich, Germany

Al-doped cubic-Li7La3Zr2O12 (Al-LLZO) is a promising solid electrolyte material for all-solid-state batteries (ASSBs). However, Al-LLZO shows a poor performance in practice mainly due to a high resistance, particularly at the electrolyte/electrode interfaces. Interfacial and lattice mismatch induced strain is a key factor in controlling the rate performance of ASSBs. In this presentation, I will discuss the influence of strain on the mechanism and conductivity of Li ion transport in Al-LLZO using DFT-based thermodynamics of defects and ab initio molecular dynamics. Our calculations on the formation energy (concentration of carriers) and migration barrier (mobility of carriers) of ions in Al-LLZO will be presented. Furthermore, by comparing PBE and HSE06 results, the effect of XC correlation functional on the stability and defect chemistry of Al-LLZO will be discussed. The results of this work can be an important step toward understanding the effect of strain on the rate capability of ASSBs.

MM 27.11　Wed 17:45　H44

Ab initio study of tetragonal and trigonal bcc-fcc transformations in Ti-Al-Mo system — •Neda Abdoshahi[1], David Holec[1], Martin Friák[2], and Mojmir Šob[2] — [1]Department of Materials Science, Montanuniversität Leoben, Franz-Josef-Strasse 18, A-8700 Leoben, Austria — [2]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Žižkova 22, CZ-616 62 Brno, Czech Republic

Motivated by a recently reported martensitic transformation in the Ti-Al-Mo intermetallic system, we employed first principles calculations to study this process on an atomic level. Our calculations reveal a spontaneous transformation from the unstable β o (bcc ordered) to the stable γ phase: there is no energy barrier along the transformation path, and an overall energy difference is *140 meV/at. for β o * γ. It is further shown that a chemical disorder reduces the driving force (total energy difference) for the β * γ dis transformation to essentially "zero" and introduces a small energy barrier of about 10 meV/at..

Next we have investigated a trigonal transformation path, connecting bcc, simple cubic (sc) and fcc structures. Not only it yields a high energy barrier of * 890 meV/at. for β 0 * γ * transformation, but it also leads to another fcc-based ordered binary compound, namely the L1 2 structure (γ *) instead of the true TiAl L1 0 (γ) ground state. Consequently we exclude the trigonal transformation path for the MTs in TiAl. In the final part we explore the impact of Mo on the stabilization of the β/β o TiAl with respect to the γ phase.

MM 27.12　Wed 18:00　H44

An *ab initio* perspective on reversible martensitic transformations in Ti-Ta shape memory alloys — •Alberto Ferrari[1], Davide G. Sangiovanni[1,2], Jutta Rogal[1], and Ralf Drautz[1] — [1]Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, 44801 Bochum, Germany — [2]Department of Physics, Chemistry, and Biology (IFM), Linköping University, SE-58183 Linköping, Sweden

Shape memory alloys exhibit reversible martensitic transformations (MTs) when temperature or stresses are applied. Modelling these transformations from first principles is not trivial, since static calculations are usually not sufficient to explore the most important aspects of the MTs, such as the Ehrenfest order of the phase transitions, the range of stability of the low- and high-temperature phases, and their free energy barrier. In this contribution, a fully *ab initio* strategy to characterize MTs in alloys is presented. The temperature dependent order parameters of a MT are calculated with *ab initio* molecular dynamics; then, the free energy of the MT, from which all the relevant thermodynamic properties of the MT can be derived, is modelled with a Landau polynomial expansion. The parameters of this expansion are completely extracted from first principles. This approach is applied to the high-temperature shape memory alloy Ti-Ta, for which very small values for the free energy barrier and the region of metastability are observed.

MM 28: Topical session (Symposium MM): Correlative and in-situ Microscopy in Materials Research

Sessions: Complex and Disordered Materials I and II

Time: Wednesday 15:00–17:45　　　　　　　　　　　　　　　　　　　　Location: H45

Topical Talk　　　　　　　　MM 28.1　Wed 15:00　H45

Towards understanding dislocation based plasticity in high entropy alloys by in-situ TEM — •Gerhard Dehm — Max-Planck-Institut für Eisenforschung GmbH

Dislocation-based deformation mechanisms of high entropy alloys (HEAs) remain elusive and require a fundamental understanding in order to tailor their mechanical properties. Since HEAs have five or more constituent elements close to the equiatomic ratio with a stable single phase, their plastic deformation is expected to be different compared to conventional alloys. Here, we present a study correlating the microstructure and dislocation plasticity of a single crystalline FeCrCoMnNi FCC single phase HEA by employing in-situ transmission electron microscope (TEM) compression and tensile deformation. Moreover, an atomic-scale chemical analysis is conducted by aberration-corrected scanning TEM energy dispersive X-ray spectroscopy (STEM-EDS) and atom probe tomography to investigate chemical inhomogeneity, for example, precipitate formation or local inhomogeneity. The aims of the study are understanding of dislocation plasticity in a FCC HEA, investigation of nanometer-scale elemental distribution and measurement of mechanical properties of FCC HEA submicron pillars. Acknowledgements: Major contributions by S. Lee, W. Lu, C. Kirchlechner, R. Raghavan, Z. Li, J. Duarte, S.H. Oh, D. Raabe and C. Liebscher are gratefully acknowledged.

MM 28.2　Wed 15:30　H45

Electron beam-induced rejuvenation in amorphous TiAl during in-situ TEM deformation — Christian Ebner[1], Jagannathan Rajagopalan[2], Christina Lekka[3], and •Christian Rentenberger[1] — [1]University of Vienna, Physics of Nanostructured Materials, Vienna, Austria — [2]Arizona State University, Department of Materials Science and Engineering, Tempe, USA — [3]University of Ioannina, Department of Materials Science and Engineering, Ioannina, Greece

In-situ transmission electron microscopy (TEM) facilitates the combined study of structure and fundamental mechanical properties at the nanometer scale. With the advancement in tools, methods and evaluation the sensitivity of measurements became increased. We show that electron irradiation of amorphous TiAl thin films under external tensile stress results in structural rejuvenation and a characteristic change of the elastic properties over time as measured by the atomic-level elastic strain contained in the TEM diffraction pattern. Deeper insights into the property changes triggered by the electron beam and resulting in the observed material response are gained via classical molecular dynamics simulations. These simulations reveal a beam-induced change in quantities like mean atomic volume, potential energy and atomic vibrational mean square displacement. The direct link to the experimental data is established by the calculation of diffraction pattern based on the simulated atomic structure.

Financial support by the Austrian Science Fund FWF: I1309 is acknowledged.

MM 28.3　Wed 15:45　H45

Micro & Nanomechanics of the Superplastic Alloy Zn-22% Al - Effect of Sample Size on Ductility — •Patrick Feld-

ner, Mathias Göken, and Benoit Merle — Materials Science & Engineering, Institute I, Friedrich-Alexander-University Erlangen-Nuremberg, 91058 Erlangen, Germany

Superplastic micro & nanoforming has a great potential for a high throughput production of small-scale structural devices with complex geometries. However, it has not yet been established if the macroscopically observed superplastic behavior also persists at microscopic length scales and which fundamental processes govern structural superplasticity in metallic alloys. For this reason, the micro & nanomechanical properties of the superplastic alloy Zn-22% Al were characterized as a function of the specimen size, using nanoindentation at elevated temperatures, in situ pillar compression, as well as in situ tensile testing in a TEM. The measured local strain-rate sensitivity and apparent activation energy provided a strong evidence for superplastic like flow at the micrometer-scale. However, below a critical specimen volume a breakdown of the superplastic flow behavior is revealed, which is accompanied by a change of the apparent rate dependency. Based on the failure morphologies observed during in situ testing, this change of the rate-controlling deformation process is discussed in terms of a transition from boundary mediated ductility to boundary mediated brittleness.

MM 28.4 Wed 16:00 H45
Plasmon characteristics of shear bands in an Al88Y7Fe5 metallic glass — •Maximilian Grove[1], Martin Peterlechner[1], Harald Rösner[1], Gerhard Wilde[1], Robert Imlau[2], and Alessio Zaccone[3] — [1]Institute für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster, Germany — [2]FEI Company, Achtseweg Noord 5, 5600 KA Eindhoven, The Netherlands — [3]Department of Physics, University of Milan, Via Giovanni Celoria, 16, 20133 Milan, Italy

Shear bands were observed as a result of plastic deformation in cold-rolled Al88Y7Fe5 metallic glass. They display alternating density changes with respect to the matrix (high and low density segments) along their propagation direction. Electron Energy loss spectroscopy (EELS) was used to map the volume Plasmons of shear bands and surrounding matrix. A characteristic Plasmon energy shift of about 10-20 meV relative to the matrix was found for both high and low density segments. For precise analysis, an open source python module (Hyperspy) was utilized to fit the peak shapes by Lorentzian functions and to visualize e.g. the Plasmon energy shift, peak width and height. The experimental results are discussed with respect to the ionic density and the plasmon-phonon interaction.

30 min. break

Topical Talk MM 28.5 Wed 16:45 H45
Recent advances in in situ TEM — •Christian Kübel[1], C.N. Shyam Kumar[1,2], Simone Dehm[1], Ralph Krupke[1,2], Manuel Konrad[1], Wolfgang Wenzel[1], Ankush Kashiwar[1,2], and Horst Hahn[1,2] — [1]Karlsruhe Institute of Technology, Germany — [2]Technical University Darmstadt, Germany

In situ TEM techniques have developed tremendously during the last decade, providing direct quantitative structural and morphological information to understand reactions and processes in nanocrystalline materials in response to an external stimulus. We will illustrate some of the possibilities in situ TEM provides to develop a deeper materials understanding and discuss the challenges in interpreting in situ results using two types of experiments:
1) Mechanical deformation of nanocrystalline Pd and Au thin films,

directly imaging grain rotation and grain boundary migration during straining and relaxation, analyzing correlations between grains and a strong Bauschinger effect observed in these materials, looking at both local processes and a statistical ensemble.
2) Thermally induced growth of nanocrystalline graphene, investigating the mobility and reactions of small graphene flakes, in particular the role of defects in different types of merging and Ostwald-type ripening of graphene flakes, supported by molecular modelling.
The influence of sample preparation and, in particular, electron beam effects on processes, reactions and kinetics will be critically discussed, to derive the main materials properties from in situ TEM experiments.

MM 28.6 Wed 17:15 H45
TEM in-situ investigation of relaxation and dynamics in amorphous FeNiP nanorods — •Katharina Spangenberg, Sven Hilke, Martin Peterlechner, and Gerhard Wilde — University of Münster, Institute of Material Physics

The method of electron correlation microscopy (ECM) using transmission electron microscopy (TEM) has been presented by He et al. to investigate dynamics and relaxation phenomena at the atomic scale. Using conventional TEM tilted dark field, the method has the ability to spatially resolve the dynamical processes in the supercooled liquid region of an amorphous alloy [1]. In the present study, the influence of the electron dose rate and non-equilibrium dynamics of amorphous FeNiP in nanostructured confinement are investigated at room temperature. A minimum dose rate is estimated to ensure proper signal-to-noise ratio. Non-equilibrium dynamics were investigated and analysed using the time autocorrelation function g2 (Δt) which can be fitted using a Kohlrausch-Williams-Watt (KWW) expression. ECM is used to calculate spatial distributions of relaxation times, represented by τ-maps. The FeNiP glass exhibits a phase separation, e.g. upon heat treatment. EDX measurements reveal a homogeneous composition or a bamboo structure of amorphous Fe-rich and Ni-rich layers. By comparing the atomic fluctuations with the local phase composition, a relation between phase separation and the time scales of the heterogeneous dynamics can be discussed.
[1] P. Zhang, J. J. Maldonis, Z. Liu, J. Schroers, & P. M. Voyles, Nature communications, 9(1), 1129, 2018

MM 28.7 Wed 17:30 H45
Fluctuation electron microscopy on PdNiP — •Farnaz Abdollahzadeh Davani[1], Sven Hilke[1], Harald Rösner[1], David Geissler[2], Annett Gebert[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Institute for Complex Materials (IKM) Leibniz-Institute for Solid State and Materials Research Dresden (IFW Dresden), Dresden, Germany

Metallic glasses are of interest due to their high strength and hardness. Plastic deformation at low and moderate temperatures is known to lead to localized shear with the formation of so-called shear bands. In this work, a Pd40Ni40P20 bulk metallic glass (BMG) was produced by ingot copper mold casting in a melt spinner under argon atmosphere. Plastic deformation of differently center edge notched beams was imposed under 3-point bending and in-situ monitored by optical microscopy. Undeformed and deformed states are compared using conventional and scanning transmission electron microscopy including high-angle annular dark-field imaging. Nano-beam diffraction patterns were collected and analyzed using variable resolution fluctuation electron microscopy. New insights with respect to structural changes induced by plastic deformation in bulk metallic glasses are discussed.

MM 29: Microstructure and Phase Transformations

Sessions: Microstructure and Phase Transformations I and II

Time: Wednesday 15:00–18:15   Location: H46

MM 29.1   Wed 15:00   H46

Abnormal grain growth in friction stir welded aluminium with zirconium additives — •Moritz Winter[1], Maximilian Gnedel[1], Amanda Zens[2], Ferdinand Haider[1], and Michael F. Zäh[2] — [1]Chair for Experimental Physics I, University of Augsburg, Universitätsstraße 2, 86159 Augsburg (Germany) — [2]Institute for Machine Tools and Industrial Management, Technical University of Munich, Boltzmannstraße 15, 85748 Garching (Germany)

Friction Stir Welding (FSW) is a well-established solid-state joining process for materials such as aluminium. In Al-Li-Cu alloys, such as AA2195 aluminium, abnormal grain growth (AGG) can be a crucial issue during post-processing of the produced welds, whilst the alloy contains zirconium for grain boundary stabilisation. Both, the microstructural stability during subsequent heat treatment as well as the mechanical properties in general can be optimized by intermixing specific micrometer-sized metal powders as well as metal foils. By dispersing additional zirconium powder inside a matrix of AA2195 aluminium during FSW, the formation of abnormal grains can be reduced, if suitable processing parameters are used. Using optical microscopy, the reduction of the secondary recrystallized area can be revealed. In addition, the formation of intermetallic phases, acting as pinning particles to hinder AGG, can be evaluated using transmission electron microscopy (TEM). Furthermore, electron backscatter diffraction (EBSD) provides insights on the changes of the crystallographic texture of the welding regions both post-weld and after subsequent heat treatment.

MM 29.2   Wed 15:15   H46

Reverse engineering the kinetics of grain growth from time-resolved 3DXRD measurements — •Mingyan Wang[1], Jules M. Dake[1], Søren Schmidt[2], and Carl E. Krill III[1] — [1]Ulm University, Germany — [2]Technical University of Denmark, Denmark

Though grain growth has been studied in polycrystalline materials for many years, our understanding of the underlying mechanisms remains incomplete. Even in the case of normal grain growth, computer simulations differ significantly from experimental findings. Instead of modeling this phenomenon using boundary parameters derived from physical principles, we decided to try out the opposite approach: that is, to work backwards from experimental measurements to the kinetics of boundary migration. Employing 3D x-ray diffraction (3DXRD) microscopy, we investigated grain growth in two different Al alloys. In a series of microstructural snapshots taken between isothermal annealing steps, we followed the morphology, misorientation and migration of thousands of grain boundaries (GBs) in a single sample. The results enable us to extract the dependency of reduced mobility (the product of GB mobility and energy) on GB misorientation. In one particular specimen, this dependency is consistent with expectations for normal grain growth, but, in the other case, we find evidence for abnormal kinetics that do not fit standard models.

MM 29.3   Wed 15:30   H46

Kinetic analysis of the precipitation sequence in dilute Al-Mg-Si alloys based on isothermal in-situ high-precision dilatometry measurements — •Robert Enzinger, Elisabeth Hengge, Wolfgang Sprengel, and Roland Würschum — Institute of Materials Physics, Graz University of Technology, Graz, Austria

The precipitation sequence in a dilute Al-Mg-Si alloy is studied utilizing recent progress in high-precision isothermal dilatometry, which yield access to tiny relative length changes $\Delta L/L$ in the range of 10^{-5} that occur on long time scales exceeding 10^5 s during isothermal ageing. For each forming phase, $\Delta L/L$-contributions arise from the volume excess due to the precipitates and the contraction of the matrix upon precipitation of solute atoms. In this way, the metastable coherent β''- and the semi-coherent β'-phase as well as the stable incoherent β-phase could unambiguously be detected on an absolute scale [1]. Reaction-rate analyses of the $\Delta L/L$ measurements based on the Johnson-Mehl-Avrami-Kolmogorov model yield the kinetic parameters for the formation of the β''-phase and either its transformation to or the formation of the β'-phase. By compiling all these findings, the industrial highly relevant time-temperature-precipitation diagrams be-

come easily accessible, which for these types of alloys were so far hard to ascertain with common experimental techniques.

[1] E. Hengge, R. Enzinger, M. Luckabauer, W. Sprengel, and R. Würschum, Phil. Mag. Lett. (2018), DOI: 10.1080/09500839.2018.1542170

MM 29.4   Wed 15:45   H46

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

Friction Stir Processing (FSP) is an established method for modifying properties in materials such as aluminium. Furthermore, the composition of the alloy can be changed by this technique. Intermixing specific micrometer-sized metal powders as well as metal foils helps to optimize both the microstructural stability during subsequent heat treatment, as well as the mechanical properties in general. Dispersing copper powder inside a matrix of AA1050 aluminium by FSP can produce a homogenous solid solution of the two elements, if suitable processing parameters are used. A substantial hardening effect is shown, due to both factors, refinement of the grain structure and solid solution hardening. By calculating the diffusion length and using the results of investigations based on energy-dispersive X-ray spectroscopy (EDS), it can be shown that the dissolution is mainly mechanically driven and not due to diffusion. Furthermore, transmission electron microscopy (TEM) provides insights on the formation of intermetallic phases during FSP, as well as after subsequent, targeted heat treatment. The results can be used in future studies to evaluate the properties of such highly deformed non-equilibrium alloys.

MM 29.5   Wed 16:00   H46

Study on nucleation rates and nucleation parameters of binary alloys — •Manoel da Silva Pinto, Martin Peterlechner, and Gerhard Wilde — Institute of Material Physics, Münster, Germany

Nucleation has an importance in diverse phenomena studied in a broad range of scientific areas. In material science, topics of special interest are, among others, new phase nucleation in alloys, solid-liquid interface energies, glass formability and possible formation of new phases in deep undercooled melts. Yet, only a few data is available on the general behavior of nucleation in alloy melts. With the help of a statistical approach related to survival analyses applied to calorimetric data of deeply undercooled alloys, we measure and analyze the nucleation rates of Au-Ge and Cu-Ge alloys for different compositions. Further parameters can be derived from this data and a comparison with the theoretical predictions from the classical nucleation theory of pure metals can be made. A dimensionless solid-liquid interface energy, the so called Spaepen factor, is determined in order to gather information about the possible nucleating phases. As a quantity depending on the crystallographic structure of the lattice formed during nucleation, the Spaepen factor could be used to describe the most probable nucleating phase and therefore the nucleation behavior in alloy melts.

MM 29.6   Wed 16:15   H46

Connectivity evolution during coarsening of nanoporous gold via kinetic Monte Carlo simulations — •Yong Li[1,2], Bao-Nam Dinh Ngô[2], Jürgen Markmann[1,2], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — [2]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

This study is motivated by controversial findings on the change of network connectivity in nanoporous gold (NPG) during coarsening. We used on-lattice kinetic Monte Carlo simulations to study the evolution of size and ligament connectivity of spinodal-like initial microstructures during coarsening. Samples with different solid volume fractions were investigated at temperatures below and above their roughening tran-

sition temperature. Based on the simulation data, we discuss which measure for size is most fundamentally linked to the coarsening kinetics. We also show that the evolution of the connectivity depends sensibly on the solid fraction. This has ramifications for how mechanical properties of nanoporous metals vary when the ligament size is tuned through coarsening.

15 min. break

MM 29.7   Wed 16:45   H46

Fractal abnormal grain growth in nanocrystalline $Pd_{90}Au_{10}$: an experimental study of factors influencing interface fractality — •Christian Braun[1], Raphael Zeller[2], Hanadi Menzel[1], Nils Boussard[1], Jörg Schmauch[1], Carl E. Krill III[2], and Rainer Birringer[1] — [1]Experimental Physics, Saarland University, Germany — [2]Institute of Functional Nanosystems, Ulm University, Germany

With grain sizes below 100 nm, nanocrystalline materials are characterized on the one hand by beneficial properties like high strength, while, on the other hand, being thermally unstable. Grain growth generally starts at temperatures that are significantly lower than usual, and microstructural coarsening often proceeds in an abnormal manner. In nanocrystalline $Pd_{90}Au_{10}$ alloys prepared by inert gas condensation, such abnormal growth leads to an impinged state of grains exhibiting highly irregular shapes, the perimeters of which are characterized by a box-counting fractal dimension of about 1.2.

Insight into the growth mechanism(s) underlying these observations could potentially be gained from a detailed analysis of interface fractality, provided the following questions can be answered: Does self-similarity in grain morphology start from the elementary building blocks of the initial microstructure (i.e., individual nanograins) or at a larger length scale? Does the fractal dimension of an abnormal grain boundary differ between its mobile and impinged states? For both questions, it is important to assess the influence of the Au concentration on abnormal grain nucleation and boundary fractality.

MM 29.8   Wed 17:00   H46

Fractal abnormal grain growth in nanocrystalline $Pd_{90}Au_{10}$: a simulation study comparing possible mechanisms — •Raphael A. Zeller[1], Christian Braun[2], Mingyan Wang[1], Rainer Birringer[2], and Carl E. Krill III[1] — [1]Institute of Functional Nanosystems, Ulm University, Germany — [2]Experimental Physics, Saarland University, Germany

Although the phenomenon of grain growth is well understood in samples having micrometer-sized grains, our understanding of the corresponding process in nanocrystalline materials is rudimentary at best. At the nanoscale the dominant mode of coarsening appears to be abnormal in nature, with a few grains growing orders of magnitude larger than their neighbors. In samples of nanocrystalline $Pd_{90}Au_{10}$ produced by inert gas condensation, microstructural coarsening is doubly abnormal, with the rapidly growing grains observed to send forth "tentacle" into the matrix, quickly encircling nearby grains and then consuming them. The perimeters of the resulting grains resemble those of fractal objects. Recent experiments suggest two possible mechanisms for fractal abnormal grain growth: (1) coalescence via grain rotation or (2) migration according to highly anisotropic grain boundary (reduced) mobilities. By combining a phase field model for boundary migration with boundary-specific selection rules, we have developed a "hybrid" simulation algorithm for each of these scenarios. A comparison of computational results with experiment reveals that one of the proposed mechanisms does a better job than the other at capturing the main features of fractal abnormal grain growth.

MM 29.9   Wed 17:15   H46

Formation and evolution of silver clusters in nanoporous gold: Views from kinetic Monte Carlo simulations — •Bao-Nam Dinh Ngô[1], Yong Li[2], Jürgen Markmann[1,2], and Jörg Weissmüller[1,2] — [1]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany

Nanoporous gold (NPG) made by dealloying assumes the geometry of an interconnected network of nanoscale ligaments. Thanks to its abundant free surface, the material offers a wide range of potential applications in actuation, catalysis, and sensing. While the fabrication process gives rise to a mostly monolithic network structure, the

small remnant of silver content proves to have strong influences on the performance of the material at work. Here, using on-lattice kinetic Monte Carlo simulations, we systematically study the formation and evolution of silver clusters at different stages of dealloying as well as during the subsequent post-dealloying coarsening. We then explore the role of dealloying potentials on the size and number of silver clusters. Finally, we briefly discuss how the environment influences the surface concentration of silver in NPG.

MM 29.10   Wed 17:30   H46

How material structure and properties of Al-Cu Friction Stir Welding seams depend on process parameters — •Roland Marstatt[1], Amanda Zens[2], Sophie Grabmann[2], Michael Friedrich Zaeh[2], and Ferdinand Haider[1] — [1]Chair for Experimental Physics I, University of Augsburg, Universitätsstraße 2, 86159 Augsburg, Germany — [2]Institute for Machine Tools and Industrial Management (iwb), Technical University of Munich, Boltzmannstraße 15, 85748 Garching, Germany

Joining of different metals, for instance of aluminium and copper, is of great industrial interest for applications in light weight construction and electromobility. In contrast to fusion welding techniques, Friction Stir Welding (FSW) does not form a multitude of brittle intermetallic phases upon joint solidification. Only a small layer of intermetallic phases is formed at the interface. Those layers are in the nanometer regime and are the key joining mechanism. In this study, the material structure, especially the intermetallic interface layers, of Al-Cu lap joints are compared with respect to variations of several welding parameters. Therefore aluminium and copper had been welded in temperature controlled mode as well as constant rotational speed mode. The set temperature respectively the set rotational speed had been varied over the possible process window. Also tool velocity, tool length and seam geometry had been varied. The structure of the intermetallic layers, especially its thickness, was measured by electron microscopy and compared to the results of corresponding shear tensile tests with respect to the process variations.

MM 29.11   Wed 17:45   H46

Impact of an Effective Triple-line Energy on the Reactive Wetting of Micro-solder on Miniaturized Cu/Ni Tracks — •Samuel Griffiths and Guido Schmitz — Institute for Materials Science, Stuttgart University, Germany

Micro-solder technologies are ubiquitous in modern electronics industries. Although these industries have driven vast practical advancements in solder technologies, little is understood about the impact of miniaturization on the reflow behaviour of solder on metal conductive tracks.

This work quantifies and analyzes the reflow behavior of Sn-based micro-solder on micro-structured Cu and Ni capillary tracks for various track widths, where solder-reflow experiments have been conducted at 350 °C in a reducing flux environment. We show evidence of an effective triple-line energy (~700 mJ/m) which impacts on the steady state system pressure and quantitatively link the triple-line energy to the solder contact angles. The steady state angle at the solder front is compared with a traditional sessile drop wetting angle measurement and, a systematic deviation is observed and discussed.

A scaling-down of the capillary track size down to a few micrometer leads to the interesting case where the track dimensions approach the size of individual substrate grains, thus requiring a modified model for describing the reflow behavior. Electron microscopic imaging and chemical analysis as well as theoretical modelling based on surface, interface and triple-line energy minimization are applied to support our conclusions.

MM 29.12   Wed 18:00   H46

Aging Processes in an Al(Mg,Si) Alloy Studied by Positron Annihilation Lifetime Spectroscopy — •Laura Resch, Gregor Klinser, Robert Enzinger, Elisabeth Hengge, Wolfgang Sprengel, and Roland Würschum — Institute of Materials Physics, Graz University of Technology, Graz, Austria

Despite the great relevance of age hardenable aluminium alloys, the atomistic processes, i.e. the formation of precipitations, underlying the age hardening are not fully understood yet. Especially, for the investigation of the initial stages and the sequence of precipitation, positron-electron annihilation has been proven to be a very suitable tool. In the present study[1] the specific technique of positron annihilation lifetime spectroscopy is applied to investigate artificial aging of the commercial Al(Mg,Si) alloy (EN-AW6060). On short timescales a

variation of the positron lifetime is observed, which is correlated with a characteristic increase in length, as monitored by in-situ dilatometry. Furthermore, the well-known aging characteristics of the hardness turned out to be directly related to the positron data. The results give hints on the early cluster formation processes. This kind of investigation allows comprehensive analyses of the aging of aluminium alloys

within different time scales as well as temperature regimes, which is important for the development of novel, tailored commercial light weight alloys.

[1] L. Resch, G. Klinser, E. Hengge, R. Enzinger, M. Luckabauer, W. Sprengel, R. Würschum, Journal of materials science 53, 14657(2018).

MM 30: Invited talk Butz

Time: Wednesday 18:15–18:45   Location: H43

Invited Talk   MM 30.1   Wed 18:15   H43
Advanced *in situ* Electron Microscopy for targeted Battery Development — ●Benjamin Butz — Micro- and Nanoanalytics Group (LMN) & Micro- and Nanoanalytics Facility (MNaF), University of Siegen, Siegen, Germany — Department of Materials Science and Engineering, Stanford University, Stanford, USA

To master the global challenges in energy storage, e.g., for e-mobility, mobile and medical devices, power tools and decentralized energy supply, novel battery concepts with enhanced energy density, long-term stability and safety at reduced price are needed. Therefore, novel technological strategies as well as capable electron-microscopic techniques along the length-scales down to the atomic regime are required to handle materials based on highly reactive species such as the alkali el-

ements. The microstructural characterization of cell parts, interfaces and starting materials commonly fails because the native state of those reactive materials is hardly preserved during sample preparation under ambient conditions or even in the high vacuum of common microscopes. The first part of this contribution will introduce cryo-EM techniques, well known from the life sciences, in conjunction with elaborated inert-gas transfer routines, which allow for detailed SEM and TEM investigation for a deep understanding of structure formation, degradation and failure. The second part will outline advanced *in situ* electrochemical and environmental TEM studies allowing for the detailed analyses of charge/discharge and corrosion/passivation processes of individual battery nanostructures and at interfaces. (This research was partially funded by the DFG under grant no. BU 2875/2-1.)

MM 31: General Meeting of the Metal- and Materials Division and Best Poster Award

Time: Wednesday 19:00–20:00   Location: H43
Duration 60 min.

MM 32: Invited talk Eberl

Time: Thursday 9:30–10:00   Location: H43

Invited Talk   MM 32.1   Thu 9:30   H43
The Digital Transformation in Materials Science and Solid State Physics — ●Chris Eberl et al. — Fraunhofer IWM. Wöhlerstr. 11, 79346 Freiburg — Albert-Ludwigs-Universität, Georges-Koehler-Allee 078, 79110 Freiburg

The Digital Transformation increasingly impacts society as a whole, even if future developments are still difficult to predict. Nevertheless, it is already obvious that data and information is becoming increasingly available across domains or disciplines through Open Data initiatives, sophisticated analytical tools, machine learning and artificial intelligence and simply 'connected apps'. Furthermore, validated physics based material models and statistical representations (e.g. generated by machine learning, artificial intelligence) allow to predict the future

behavior and perform status updates in real time. As a result, increasingly complex interrelationships can be accessed. Last but not least, the increasing data flow associated with this development, have led to projects which aim to structure and standardize data and information by the use of a common ontology and use knowledge graph-based databases. However, the real potential will be unfolding when these tools and infrastructure are combined and integrated in a seamless way. Within this talk, examples will be shown of how the integral use of physics and data based modelling can be used and how it is changing experimental approaches. In the future, we might be able to develop complex relationships between manufacturing processes, properties and materials behavior under various load conditions (e.g. online lifetime assessment coupled with predictive maintenance).

MM 33: Topical session (Symposium MM): Big Data Analytics in Materials Science

Sessions: Big Data Analytics in Materials Science I and II

Time: Thursday 10:15–13:15   Location: H43

Topical Talk   MM 33.1   Thu 10:15   H43
Supervised and unsupervised learning from the large body of materials literature — ●Gerbrand Ceder — University of California, Berkeley, CA, USA

The overwhelming majority of scientific knowledge is stored as unstructured text in millions of publications. I will show some results showing how knowledge can be extracted from such a large corpus of text using a combination of Natural Language Processes (NLP) combined with Machine Learning (ML). NLP is necessary to turn the unstructured information in the scientific literature into structured data on which ML can operate. As an example, I will demonstrate how a vector representation of words can capture inorganic materials science concepts from 3.3 million scientific abstracts without human labelling or supervision. Remarkably, such basic text-based methodology can be used to

make predictions of new materials, the properties of which we verify with Density Functional Theory. An alternative and more complex example will be discussed whereby all materials synthesis information is extracted from several million papers. Constructing synthesis recipes from papers requires extremely high precision and recall of relevant chemicals and operational procedures. I will show how this can be achieved by combining various supervised and unsupervised machine learning methods to create the largest data set of solid-state synthesis reactions.

MM 33.2   Thu 10:45   H43
Reproducible massive calculations and data sharing with Ai-iDA and the Materials Cloud — ●Giovanni Pizzi[1], Leopold Talirz[1], Snehal Kumbhar[1], Aliaksandr Yakutovich[1], Elsa Passaro[1], Marco Borelli[1], Sebastiaan P. Huber[1], Mar-

tin Uhrin[1], Spyros Zoupanos[1], Fernando Gargiulo[1], Ole Schuett[2], Joost VandeVondele[3], Thomas C. Schulthess[3], Berend Smit[1], and Nicola Marzari[1] — [1]NCCR MARVEL and EPFL, CH — [2]Empa, Switzerland — [3]CSCS and ETHZ, CH

We discuss the challenges and solutions to store data resulting from the modern, complex workflows of computational science, allowing for the search and dissemination of results according to the FAIR principles of sharing. We first show how a materials' informatics framework like AiiDA [1] allows to automate all calculations and store their entire provenance. By uploading all data to the Materials Cloud (materialscloud.org), results can be disseminated seamlessly, DOIs are assigned to the datasets, and interactive (online or local) browsing of the provenance makes it possible to explore any element of the workflow guaranteeing its full reproducibility and enabling reuse of the results. Materials Cloud also provides intuitive web-based simulation services based on AiiDA, reducing the access barrier to HPC simulation tools.

[1] G. Pizzi et al., Comp. Mat. Sci. 111, 218 (2016), www.aiida.net

MM 33.3　Thu 11:00　H43

The NOMAD 2018 Kaggle Competition: Tackling Materials-Science Challenges through Crowd Sourcing — •Christopher Sutton[1], Luca M. Ghiringhelli[1], Takenori Yamamoto[2], Xiangyue Liu[1], Angelo Ziletti[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Institute for Mathematical and Computational Sciences, LLC Yokohama, Japan

Machine learning (ML) promises to accelerate the discovery of novel materials by screening candidate compounds at significantly lower computational cost than traditional electronic-structure approaches. However, it is often *a priori* unclear which ML models are suitable for a given problem and optimizing a model can be a time-consuming endeavor. Crowd sourcing allows for comparing several ML models by identifying a key problem and challenging the community to solve it. To this end, the Novel Materials Discovery (NOMAD) Centre of Excellence together with Kaggle - one of the most well known hosting platforms - organized an open data-science competition to predict two key properties of transparent conducting oxides (TCOs): band gap energy (for transparency) and formation energy (for stability). Although these materials are crucial for optoelectronic devices, only a small number TCOs are currently known. In this contribution, we present the winning model out of nearly 900 participants based on a novel crystal-graph representation and an analysis of the relative importance of representation vs regression model for the performance of several ML approaches.

MM 33.4　Thu 11:15　H43

Symmetry-invariant basis representations for machine- learning of electronic structure data beyond energies — •Michael Luya[1,2] and Reinhard J. Maurer[2] — [1]Department of Mathematics, University of Warwick, Coventry, United Kingdom — [2]Department of Chemistry, University of Warwick, Coventry, United Kingdom

Recent successes on the high-dimensional machine-learning-based (ML) interpolation of total energies and forces from ab-initio computations are extremely encouraging for the future role that machine-learning can play in condensed matter simulation and electronic structure theory. Beyond scalar energy fields, ML can be useful to find efficient representations of quantum mechanical interaction integrals and Hamiltonians in atomic orbital basis representations. These represent tensor fields, which, contrary to scalar fields, feature covariance properties and additional directional coordinate dependence that need to be addressed.

Here we present an approach based on a generalisation of Slater-Koster transformation and symmetry-adaptation to transform interaction integrals and Hamiltonians from electronic structure theory in atomic-orbital representation into rotationally invariant forms that are amenable to established machine learning methods. We validate our approach on a large set of training data on simple organic molecules of varying size.

15 min. break

Topical Talk　　　　　　　MM 33.5　Thu 11:45　H43

Extending high-throughput materials discovery to finite temperatures: Concepts and application — •Tilmann Hickel[1], Janssen Jan[1], Halil Sözen[1], Fritz Körmann[1], Sudarsan Surendralal[1], Mira Todorova[1], Yury Lysogorskiy[2], Ralf Drautz[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany — [2]Atomistic Modelling and Simulation, ICAMS, Ruhr-Universität Bochum, D-44801 Bochum, Germany

Present ab initio based high-throughput methods are commonly restricted to T=0 K calculations. For many technologically relevant materials, however, properties and thermodynamic stability drastically change for finite temperatures. Recent developments allow us to calculate thermodynamic quantities up to the melting point, but require complex simulation protocols that couple computer codes from various disciplines together with advanced mathematical algorithms. To provide a platform to develop, implement, test and apply such protocols we have created a Python based integrated development environment called pyiron. After highlighting the underlying algorithmic concepts, we use the example of the hard-magnetic material system Ce-Fe-Ti to demonstrate the materials scientific consequences. Using high throughput screening we study how adding further elements impacts relative phase stabilities at finite temperatures and thus partitioning. This yields design criteria that extend the chemical composition space to quaternary, more stable hard magnetic materials.

MM 33.6　Thu 12:15　H43

Crystal-structure identification in polycrystals via Bayesian deep learning — •Angelo Ziletti, Andreas Leitherer, Matthias Scheffler, and Luca Ghiringhelli — Fritz Haber Institute of the Max Planck Society Faradayweg 4-6 14195 Berlin, Germany

Thanks to open-access online computational repositories (e.g. http://nomad-coe.eu) and experiments (e.g. atom probe tomography), researchers have now access to a vast amount of three-dimensional structural data. To extract valuable information for materials characterization and analytics, computational methods that automatically and efficiently detect long-range order are needed. Current methods are either not stable with respect to defects, or base their representation on local atomic neighbourhoods, which in turn makes it difficult to detect "average" longe-range order. In the proposed approach, for a given crystal structure, we simulate its (three-dimensional) diffraction pattern, and by means of a spherical-harmonics expansion, we compute a rotationally and translationally invariant representation. A convolutional neural network is then used to identify the correct crystal structure; in particular, we use a Bayesian neural network in order to obtain statistically-principled classification probabilities and model uncertainty. This methodology is used to classify grains in polycrystals, find coherent regions in amorphous solids, but also detect crystallographic defects such as twin boundaries, stacking faults, and edge dislocations in heavily defected crystal structures.

MM 33.7　Thu 12:30　H43

Neural-network representation of materials for robust crystal-structure recognition — •Andreas Leitherer, Angelo Ziletti, Matthias Scheffler, and Luca M. Ghiringhelli — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Assigning the crystal structure to local regions of large atomic structures can reveal hidden patterns and thus interesting material properties. Available computational methods either support a large number of space groups but show critically limited robustness, or are very robust but can treat only a handful of classes. We use neural networks to robustly assign the correct crystal-structure type to a given material while being able to treat numerous space groups and chemical species. To capture information about the local chemical environments, we apply the smooth-overlap-of-atomic-positions (SOAP) descriptor, serving as input to the deep-learning model. Since the neural network provides an intrinsic similarity metric, we are able to investigate structural transitions such as the Bain path between face-centered cubic and body-centered cubic structures. We also discuss the application of our framework to detect precipitates in Ni-based superalloys (materials used in aircraft engines), whose structure is usually experimentally investigated via atom probe tomography. Finally, we show that the neural network automatically learns how to map crystal structures to a meaningful low-dimensional manifold, an ability which we exploit by building easily interpretable structural-similarity maps.

MM 33.8　Thu 12:45　H43

Artificial intelligence in materials science: towards optimal descriptors — •Benedikt Hoock[1,2], Santiago Rigamonti[1], Luca Ghiringhelli[2], Matthias Scheffler[1,2], and Claudia Draxl[1,2] — [1]Humboldt-Universität zu Berlin, Berlin, DE — [2]Fritz-Haber-Institut der MPG, Berlin, DE

Materials data contained in repositories like NOMAD [1] can be exploited in many useful ways, such as to better understand existing materials or to discover new materials with desired properties. A crucial step towards these goals is to find a set of meaningful descriptors, i.e. parameters based on computationally cheap input data that capture the physical mechanisms underlying certain material properties. In this work, we develop principles for constructing up to millions of candidate descriptors from simple physical properties. These principles involve mathematical operations [2] and different averaging procedures considering the local ordering. We compare two compressed sensing methods, LASSO+ℓ_0 [2] and SISSO [3], at identifying optimal descriptors out of all the candidates. Likewise, we introduce and compare cross-validation based model-selection strategies that use either the average training or the average test error as a criterion, aiming at increasing the descriptors' generalizability. We use two ab initio data sets, comprising group-IV zincblende ternaries and transparent conducting oxides, to test this methodological approaches.

[1]: C. Draxl & M. Scheffler, MRS Bulletin, 43, 676 (2018).
[2]: L. M. Ghiringhelli, et. al., Phys. Rev. Lett. 114, 105503 (2015).
[3]: R. Ouyang, et. al., Phys. Rev. Mater. 2, 083802 (2018).

MM 33.9 Thu 13:00 H43
Global sensitivity analysis and surrogate modeling for ma- terials models with rapid local variations — Juan Lorenzi[2], Sandra Döpking[1], and •Sebastian Matera[1] — [1]Institut f. Mathematik, Freie Universität Berlin — [2]Lehrstuhl F. Theoretische Chemie, Technische Universität München

Most material models depend on a number of input parameters which carry some uncertainty. Quantifying the impact of these errors on the model output is the purpose of global uncertainty and sensitivity analysis. This requires some kind of sampling of the parameter space and surrogate modeling has become a popular tool to lift the problem of repetitive, computationally expensive model evaluations. Surrogate modeling becomes challenging when the underlying model shows locally rapid variations, e.g. if a materials model exhibits a phase transition within the parameter domain. We present a modification of the classical Shepard interpolation, which has been designed for such problems. This approach employs a local, node specific distance metric instead of a global metric and uses error estimates for the superposition of different local linear models at a query point. We demonstrate the approach on the global sensitivity analysis of a stochastic model for CO oxidation, which has been parametrized using Density Functional Theory. We find that we can obtain reasonably accurate estimates of the sensitivity indices already at a modest number of evaluations of the original high-fidelity model.

MM 34: Methods in Computational Materials Modelling (methodological aspects, numerics)

Sessions: Finite temperature properties and computational spectroscopy

Time: Thursday 10:15–13:00 Location: H44

MM 34.1 Thu 10:15 H44
Tight-binding insight in phase stabilities of magnetic iron — •Ning Wang[1], Thomas Hammerschmidt[1], Tilmann Hickel[2], Jutta Rogal[1], and Ralf Drautz[1] — [1]ICAMS, Ruhr-Universität Bochum — [2]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf

Although the phase diagram of iron has been well-established, we still lack a consistent and theoretical understanding. The difficulty lies in the modelling of complex thermal excitations including magnetic, vibrational and electronic excitations and their mutual interactions. Here we present a spin-lattice fluctuation theory by combining the spin-fluctuation theory and the semi-empirical tight-binding model. With this model we perform a thorough investigation of magnetic and structural phase transitions in magnetic iron. A thermodynamic-integration calculation shows a bcc-fcc phase transition driven by magnetic fluctuations. We employ the spin-space averaging scheme and obtain strong magnetic phonon softening in bcc iron. We observe a sign change in the calculated vibrational-entropy difference between bcc and fcc iron, which is atrributed to the transformation back from fcc to bcc iron and in a good agreement with experimental deduction.

MM 34.2 Thu 10:30 H44
The temperature dependence of surface and grain boundary energies from first principles — •Daniel Scheiber, Maxim Popov, and Lorenz Romaner — Materials Center Leoben Forschung GmbH

Material properties generally depend on temperature. While for many bulk properties, the temperature dependence has been well investigated in experiment and theory, for grain boundary and surface energies the topic has remained largely unexplored. A large gap exists between experimental measurements at elevated temperatures and ab-initio simulations performed at 0K. The explanation for these deviations could also be rooted in the missing temperature treatment in the simulations.

In this study, we investigate the temperature dependence grain boundary energies in tungsten. Within the quasi-harmonic approximation we evaluate the phonons using ab-initio density functional theory for different grain boundaries. With that the Helmholtz free energies for grain boundaries are evaluated as a function of temperature. Our simulations show considerable reduction in interface energy with temperature for all investigated grain boundaries and surfaces. This change in interface energy may be directly related to changes in segregation energy, as it is known that segregation scales with grain boundary energy. Finally, we discuss the limitations of our approach and compare the results to available experimental data.

MM 34.3 Thu 10:45 H44
***Ab initio* benchmark of anharmonic free energies in naphtalene** — •Marcin Krynski, Nathaniel Raimbault, and Mariana Rossi — Fritz Haber Insitute of the Max Planck Society, Berlin, Germany

Organic molecular crystals are a vast group of compounds with undisputed industry importance, known for their ability to form polymorphs with properties tied strongly to their crystallographic structure. A large body of theoretical research is centered on polymorph energy ranking [1], which is impacted by the (often neglected) thermodynamic conditions and anharmonicities of the potential energy surface (PES). We present a study of anharmonic contributions to the free energies of the p21a14 and p21c14 molecular crystal polymorphs of naphthalene. We employ dispersion-corrected density-functional theory and compare full anharmonic free-energy evaluations [2] to more computationally tractable approximate methods, gauging the effect of lattice expansion at different temperatures. We show that at the PES, p21c14 is lower in energy than p21a14 by ca. 3meV/molecule for any combination of PBE/PBE0/B3LYP with pairwise or many-body van der Waals (vdW) corrections. Without vdW corrections, the crystals are not stable. We assess whether temperature and lattice expansion explain the experimentally observed stability of the p21a14 polymorph and extend our methodology to polymorphs of pimelic acid, which shows a puzzling temperature-dependent lattice contraction along one axis. [1] A. Reilly *et al.*, *Acta Cryst. B* **72**, 439 (2016); [2] M. Rossi, P. Gasparotto, M. Ceriotti, *PRL* **117**, 115702 (2016)

MM 34.4 Thu 11:00 H44
Phase stability of dynamically disordered solids from first principles — Johan Klarbring and •Sergei Simak — IFM, Linköping University, SE-581 83, Linköping, Sweden

Dynamically disordered solid materials show immense potential in applications. In particular, superionic conductors are very promising as solid state electrolytes in batteries and fuel cells. The biggest obstacle in living up to this potential is the limited stability of the dynamically disordered phases. To obtain the free energies of disordered materials has long been a challenge. We outline a method that offers a solution [1]. It is based on a stress-strain thermodynamic integration on a deformation path between a mechanically stable ordered variant of the disordered phase, and the dynamically disordered phase itself. We show that the large entropy contribution associated with the dynamic disorder is captured in the behavior of the stress along the deformation path.We apply the method to Bi_2O_3, whose superionic δ-phase is the fastest known solid oxide ion conductor. We accurately reproduce the experimental transition enthalpy and the critical temperature of the

phase transition from the low temperature ground state α phase to the superionic δ phase. The method can be used for a first-principles description of the phase stability of superionic conductors and other materials with dynamic disorder, when the disordered phase can be connected to a stable phase through a continuous deformation path.

[1] J. Klarbring and S. I. Simak, Phys. Rev. Lett. 121, 225702 (2018).

MM 34.5   Thu 11:15   H44

The driving force behind the distortion of 1D monatomic chains - Peierls theorem revisited — •Daniela Kartoon[1,2], Uri Argaman[1], and Guy Makov[1] — [1]Materials Engineering Department, Ben-Gurion University of the Negev, Beer Sheva 84105, Israel — [2]NRCN-Nuclear Research Center Negev, Beer Sheva IL 84190, Israel

The onset of distortion in one-dimensional monatomic chains with partially filled valence bands is considered to be well-established by the Peierls theorem, which associates the distortion with the formation of a band gap and a subsequent gain in energy. Similar mechanism is commonly used to explain the distorted structures in half-filled p-band materials. Employing modern total energy methods on both one-dimensional chains and half-filled p-band materials, we reveal that the distortion is not universal, but conditional upon the balance between distorting and stabilizing forces. Furthermore, in all systems studied, the electrostatic interactions between the electrons and ions act as the main driving force for distortion, rather than the electron band lowering at the Fermi level as is commonly believed. The main stabilizing force which drives the materials toward their symmetric arrangement is derived from the electronic kinetic energy. Both forces are affected by the external conditions, e.g. stress, and consequently the instability of one-dimensional nanowires is conditional upon them. This suggests a more general mechanism of high-to-low symmetry transitions, and may shed new light on the distortion of more complex structures.

15 min. break

MM 34.6   Thu 11:45   H44

Anharmonic Raman Spectra in Polymorphic Crystals from Density-Functional-Perturbation Theory and Machine Learning — Nathaniel Raimbault and •Mariana Rossi — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Anharmonic contributions to vibrational Raman spectra of molecular crystals can be decisive to identify the structure of different polymorphs. In this work we characterise the low-frequency Raman spectral region of different polymorphs of the flexible aspirin and paracetamol crystals. We include anharmonicities though the time-correlation formalism, combining ab initio molecular dynamics and density-functional perturbation theory (DFPT) implemented in a full-potential, all-electron framework [1]. Lattice expansion and anharmonic thermal nuclear motion strongly affect the collective vibrations of the low-frequency region. This effect is much less pronounced at higher frequencies. We obtain excellent agreement with experimental lineshapes at frequencies below 200 cm^{-1}, highlighting the necessity of going beyond the harmonic approximation and providing unambiguous polymorph assignment. In order to bypass the cost of DFPT evaluations of the polarisability tensor, we employ different forms of Kernel Ridge Regression (KRR) and discuss their efficiency. Training our models on several hundreds of points, we reproduce Raman spectra that would otherwise require the calculation of tens of thousands of points. [1] H. Shang, N. Raimbault et al., New J. Phys. **20**, 073040 (2018)

MM 34.7   Thu 12:00   H44

Electric Field Gradient in Ca3Mn2O7 — Pedro Rodrigues[1], Ivan Miranda[2], Samuel Santos[1,2], Armandina Lopes[1], Gonçalo Oliveira[1], Lucy Assali[2], João Pedro Araujo[1], and •Helena Petrilli[2] — [1]Faculdade de Ciências, Universidade do Porto,Porto, Portugal — [2]Instituto de Física, Universidade de São Paulo, São Paulo, Brazil

Naturally layered perovskites, such as the Ruddlesden-Popper phases or A-site ordered double perovskites have appeared as a fascinating route in exploring the design and achievement of nonexpensive room temperature multiferroic materials. In these, distortions of the lattice such as octahedron rotation and tilting modes, couple to polar cation dislocation modes, inducing cation ordering and a spontaneous ferro-electric polarization, a mechanism known as hybrid improper ferroelec-

tricity. Here, several structural, charge and magnetic phase transitions of Ca3Mn2O7 is studied by combining theoretical and experimental methods, in order to provide a tool to unravel its local electronic and magnetic properties. The theoretical approach is performed using ab-inito electronic structure calculations, in the framework of the Density Functional Theory (DFT); measurements are performed for structural characterization as well as magnetic and hyperfine quantities. Through this comparison, a local scenario of the complex behavior is this class of systems is studied. By inspecting electric field gradients at the nuclei obtained via theoretical calculations and inferred from Perturbed Angular Correlations (PAC) measurements at a Cd probe, trends are obtained and the application of the proposed procedure is discussed .

MM 34.8   Thu 12:15   H44

Proton irradiation of ice in space conditions simulated via real-time TDDFT — •Daniel Muñoz-Santiburcio — CIC nanoGUNE, San Sebastián, Spain

Proton irradiation of ice is of great importance for a number of astrophysical/chemical processes. Here I will show the results of real-time TDDFT calculations where the irradiation of ice with highly energetic protons is simulated in real time via Ehrenfest MD [1], following the excitations of the electronic subsystem in the ice sample promoted by the passing of the proton projectile at the same time that the change of the trajectory of the projectile is strictly described, going beyond the 'constant velocity' approximation that is usually employed when modeling such radiation damage processes. I will also describe the dependence of these effects as a function of the energy and orientation of the incoming proton, helping to fill a gap in the current experimental and theoretical knowledge of this process.

[1] D. Muñoz-Santiburcio and E. Artacho, in preparation.

MM 34.9   Thu 12:30   H44

Computation of NMR shifts for paramagnetic solids including zero-field-splitting: significant effects beyond the contact shifts — •Arobendo Mondal[1,2] and Martin Kaupp[1] — [1]Theoretical Chemistry/Quantum Chemistry, TU Berlin, Germany — [2]Theoretical Chemistry, TU Munich, Germany

NMR is a powerful tool for studying the structural and electronic properties of paramagnetic solids. However, the interpretation of paramagnetic NMR spectra is often challenging as a result of the interactions of unpaired electrons with the nuclear spins of interest. Recently, we reported a novel protocol to compute and analyze NMR chemical shifts for extended paramagnetic solids, accounting comprehensively for Fermi-contact (FC), pseudo-contact (PC), and orbital shifts.[1] We combine periodic DFT computation of hyperfine and orbital-shielding tensors with an incremental cluster model for g- and zero-field-splitting (ZFS) D-tensors. The hyperfine tensors are computed with hybrid DFT functionals using the highly efficient Gaussian-augmented plane-wave implementation of the CP2K code. The incremental cluster model allows the computation of g- and ZFS D-tensors by ab initio complete active space self-consistent field and N-electron valence-state perturbation theory methods. We find that ^{7}Li shifts in the high-voltage cathode material LiCoPO$_4$ are dominated by spin-orbit-induced PC contributions, in contrast to previous assumptions, changing the interpretation of the shifts fundamentally in terms of covalency.

[1] Mondal, A.; Kaupp, M. J. Phys. Chem. Lett., **2018**, 9, 1480-1484.

MM 34.10   Thu 12:45   H44

Characterization of local structure using a mixed radial, orientational three-body correlation function — •Martin H. Mueser and Sergey V. Sukhomlinov — Universität des Saarlandes, 66123 Saarbrücken, Germany

Computer simulations of condensed matter systems are often run with the goal to ascertain the degree to which the local structure of a system lacking long-range order resembles that of crystalline reference phases. As a tool for such analysis we propose a mixed radial, orientational three-body correlation function, i.e., $g_{ABC}(r_{BC}, \vartheta_{ABC})$. This function is defined to be proportional to the probability of finding an atom of type C at a distance r_{BC} under an angle of ϑ_{ABC} given that r_{AB} is within 10% of a typical AB bond length or AB nearest-neighbor distance. This correlation function allows the local order in disordered systems to be more easily related to that of reference crystals than with other methods that have so far been conventionally used. This method could also be used to detect and quantify local symmetries.

In order to demonstrate the use of the analysis and its usefulness, a visual library of mono- and two-component crystals is produced and

compiled, and then applied to a diverse body of selected liquids and disordered solids. These include the analysis of the extent with which liquid Lennard-Jonesium and liquid copper resemble face-center-cubic or hexagonal close packing, the relative amount of cristobalite in a simple model of liquid silica, the extend of the Peierls deformation in liquid antimony and the identification of the seesaw molecular geometry occurring in zinc-phosphates under pressure.

MM 35: Topical session (Symposium MM): Correlative and in-situ Microscopy in Materials Research

Sessions: Surfaces and Interfaces; Thin Films and Nanostructures

Time: Thursday 10:15–13:00   Location: H45

Topical Talk   MM 35.1   Thu 10:15   H45
Friction mechanisms revealed by scanning force and electron microscopy — •Roland Bennewitz[1], Christiane Petzold[1], Marcus Koch[1], Nicholas Chan[3], SG Balakrishna[1], Philip Egberts[3], Andreas Klemenz[2], and Michael Moseler[2] — [1]INM Leibniz Institute for New Materials, Saarbrücken, Germany — [2]Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany — [3]Department of Mechanical and Manufacturing Engineering, University of Calgary, Canada

Atomic force microscopy (AFM) is a well-established imaging tool in nanoscience, in some applications with atomic resolution. Beyond imaging structure on nanometer scale, force measurements by AFM also reveal molecular-scale mechanisms of friction. As an example, we will present data for the structure and friction response of graphene layers grown epitaxially on Pt(111) surfaces. In friction and wear studies, the AFM tip is not only an imaging probe but equally important part of the sliding contact. While surface wear is revealed by AFM imaging, tip wear requires electron microscopy of the tip. We will discuss results for the tribochemical wear of tips when sliding silicon against gold.

MM 35.2   Thu 10:45   H45
Characterization of surface reactions by non-contact atomic force microscopy with functionalized tips — •Andreas Dörr[1], Maximilian Ammon[1], Van-Dong Pham[1], Milan Kivala[2], and Sabine Maier[1] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen — [2]Centre for Advanced Materials, Ruprecht-Karls-Universität Heidelberg, Heidelberg

Atomically resolved images of surface-supported molecular structures have been achieved using non-contact atomic force microscopy (nc-AFM) with functionalized tips.[1] The key step involves the attachment of suitable small molecules, e.g. CO, to achieve high spatial resolution. Submolecular resolution imaging is a versatile tool to unravel novel reaction pathways of surface-supported molecules in on-surface synthesis. Here, we present a low-temperature scanning tunneling microscopy and nc-AFM study with functionalized tips to understand the on-surface reaction of amine-functionalized carbonyl-bridged triphenylamine derivatives. On Au(111), we observe linear structures upon reaction, while on Ag(111), covalently-linked dimers are formed that connect to 2D structures at higher temperatures. However, the molecular structure of the polymerized reaction products is found to be similar on both surfaces. The nc-AFM measurements with CO functionalized tips indicate that mainly the amine-groups are involved in the polymerization reaction. We will discuss the geometric structure of the reaction products and the reaction kinetics on both surfaces.

[1] L. Gross, et al. Science 325, 1110 (2009)

MM 35.3   Thu 11:00   H45
Mesoscopic THz imaging of quantum materials - The instrument perspective — •Marc Westig, Holger Thierschmann, Allard Katan, Matvey Finkel, and Teun M. Klapwijk — Department of Quantum Nanoscience, Kavli Institute of Nanoscience, TU Delft, The Netherlands

One of the challenges in modern condensed-matter physics is the fundamental understanding and technological use of quantum materials. In these materials, strong interactions between electrons and other quasi-particles lead to emerging properties. Examples are high-temperature superconductivity, magnetism and hydrodynamic electron flow in graphene. Another effect of strong electron interactions is that different ground states compete. In the detector-relevant disordered superconductors, this leads to electronic inhomogeneity over a range of few tens of nanometers. The consequences for their local elec-trodynamics are still unknown and, hence, how the detector sensitivity is influenced.

Motivated by these challenges, we have started to develop high-frequency local probe instruments ranging from a few up to several hundred GHz. My talk will focus on the instrument side, but always keep an eye on the physical systems we envision to probe. A natural question which arises is about the image formation on the nanometer scale in such an instrument. Our approach focuses on two different probe technologies, a microstrip coupled metallic tip and a waveguide coupled dielectric tip. We will show preliminary imaging results in a disordered model system around 3 GHz.

30 min. break

Topical Talk   MM 35.4   Thu 11:45   H45
In-situ Microscopy Testing of Metallic Thin Films — •Velimir Radmilović — University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia — Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11000 Belgrade, Serbia

Despite low ductility and wear resistance as well as poor fracture toughness, silicon and silicon-nitride (Si3N4) have been widely used in fabrication of micro-electromechanical (MEMS) and nano-electromechanical (NEMS) systems. Although metallic resonators tend to demonstrate considerably higher energy dissipation in the medium frequencies band, they have been proposed as a potential substitute for Si and Si3N4 devices since metallic films offer higher electrical conductivity and superior ductility. Resonant properties of nanocrystalline MEMS and NEMS metallic devices have been investigated by means of in-situ electron microscopy mechanical testing, using near-infrared laser interferometry. Mechanical testing is performed in tandem with shape modification and microstructural characterization by focused ion beam, scanning and transmission electron microscopy. Depending on alloy chemical composition and processing parameters, metallic films transform from pure crystalline to a unique microstructure with a dense distribution of nm-scale crystallites dispersed in an amorphous matrix. These films exhibit high nanoindentation hardness, metallic conductivity and tunable residual stresses, while surfaces display smooth morphology, characteristic for sputtered amorphous films.

MM 35.5   Thu 12:15   H45
Correlative in situ microscopy studies of highly directional nanowires — •Lilian Vogl, Peter Schweizer, Mingjian Wu, and Erdmann Spiecker — FAU Erlangen-Nürnberg, IMN

Here we present a novel approach to synthesize Molybdenum oxide nanowires from Molybdenum Disulfide (MoS2) in situ, using microscopy as a direct feedback-mechanism enabling parameter optimization as well as the analysis of growth kinetics. The Nanowire Synthesis is carried out in an in situ Light Microscopy heating chamber under controlled oxygen atmosphere. This allows us to directly measure the growth rate using digital image correlation and determine the influence of temperature and pressure on the synthesis. Correlative Electron Microscopy and spectroscopy is used to characterize the crystal structure and growth direction as well as to analyze the chemical composition of the wires. The diameter of the synthesized nanowires is typically between 15 to 250 nm with a length of up to several tens of micrometers. The growth of the wires is highly directional and follows the [11-20] directions of MoS2. In Addition to the analysis of the growth behavior of the nanowires, the functional properties are elucidated. To determine the electrical properties of the wires in situ four probe measurement in an SEM are performed on the micro-scale. The U-I sweep shows a linear behavior of the nanowires corresponding to an ohmic conductor. Currently in situ bending tests and Resonance measurements are done

to evaluate the mechanical properties of the nanowires.

MM 35.6   Thu 12:30   H45

Correlative TEM and XRD study of the role of Au on the solid state dewetting behavior of Au/Ni bilayers on α-Al2O3 — •Johannes Will[1], Patrick Herre[1], Tobias Zech[1], Johanna Schubert[1], Mingjian Wu[1], Tadahiro Yokosawa[1], Jan Schwenger[1], Stefan Romeis[1], Dong Wang[2], Tobias Unruh[1], Wolfgang Peukert[1], and Erdmann Spiecker[1] — [1]FAU Erlangen-Nürnberg — [2]TU Ilmenau

In this study, we investigated the influence of Au on the structure and properties of binary Au-Ni nanoparticles (NPs) equilibrated by solid-state dewetting and subsequent quenching on (0001) oriented sapphire single crystals. We contribute to the research field by investigating the role of Au on the mechanical as well as structural properties of Au-Ni NPs by a systematic variation of the Au content. Here, our methodological approach is to combine TEM and EDXS with XRD in order to obtain complementary information about the morphology, orientation and in-plane as well as out-of-plane strain of the NPs with respect to the sapphire substrate. Furthermore, the impact of alloying and interface structure on the mechanical properties of the NPs was tested by in situ SEM compression experiments. As shown by XRD and TEM, it is possible to fabricate alloyed NPs for all investigated Au concentrations. Moreover, a pronounced in- and out-of-plane orientational relationship is demonstrated. In addition, no misfit dislocations at the NP substrate interface are present. This kind of interface is in-line with previous findings for pure Ni NPs, where it was denoted as delocalized coherent interface.

MM 35.7   Thu 12:45   H45

In situ TEM observation of phase decomposition in NiAu nanoparticles derived from solid-state dewetting of bilayer metal thin films — •Johanna Schubert[1], Christian Wiktor[1], Simon Kraschewski[1], Patrick Herre[2], Mingjian Wu[1], Wolfgang Peukert[2], and Erdmann Spiecker[1] — [1]Institute of Micro- and Nanostructure Research, FAU, Erlangen, Germany — [2]Institute for Particle Technology, FAU, Erlangen, Germany

Solid-state dewetting of multilayer metal thin films is a novel method to tailor alloy nanoparticles in composition, size, shape and orientation by varying layer thicknesses and dewetting parameters. Alloy nanoparticles produced in this way are ideal model systems for studying fundamental aspects of phase transformation in confined volumes. By dewetting of Ni-Au bilayers AuxNi1-x alloy nanoparticles with various compositions were produced. Despite a large miscibility gap in the Ni-Au system solid solution particles were obtained by fast quenching. Subsequent annealing at lower temperature allowed us to study the phase decomposition under controlled conditions. Two decomposition pathways were observed resulting in particles with Au-rich phases on the outer facets and particles with lamellar structure of alternating Ni- and Au-rich phases. In situ TEM was applied to gain deeper insight into the role of nanoparticle morphology on the mechanisms and kinetics of phase decomposition. High resolution analysis of particle cross sections revealed closely spaced 1/2[110]-typed edge dislocations at the phase boundaries. The dislocations compensate the large lattice misfit of > 10 % between the Ni- and Au-rich phases.

MM 36: Liquid and Amorphous Metals

Sessions: Local structure and crystallization; Mechanical deformation of metallic glasses

Time: Thursday 10:15–13:00   Location: H46

MM 36.1   Thu 10:15   H46

The effect of temperature and composition on resistivity of Bi-Ga and Ga-In binary alloys — •Yuri Kirshon[1], Guy Makov[1], and Eyal Yahel[2] — [1]Ben-Gurion University of the Negev, Beersheba, Israel — [2]NRCN, Beer-Sheva, Israel

The electrical resistivity of liquid metals and alloys is a probe of the electronic and structural properties of the system. The present study focused on the development of an experimental apparatus to measure the electrical resistivity of liquid metals and its application to selected metal and alloy systems. The presentation consists of two parts: the first reports on the design of the experimental measuring system, with some emphasis on the importance of component materials. The second part reports on measurements of resistivity in pure Bi, Ga and In, also, Bi-Ga and Ga-In binary alloys were tested as well. The resistivity of the alloys was measured for selected compositions over wide range of temperatures. In all the studies the absolute resistivity was determined up to an error of 3% and the results are with good agreement with previous studies. A clear linear correlation between resistivity and temperature is obtained for tested pure metals and some tested alloys. For Bi-Ga the resistivity and its temperature coefficients are found to vary smoothly with composition as suggested by simple theoretical models. In contrast, for Ga-In alloys the composition dependence is non-monotonous. In addition, the near eutectic alloys display anomaly which point toward a structural transition in the liquid.

MM 36.2   Thu 10:30   H46

Impact of Glass Transition on Crystallization Kinetics of Phase-Change Material Ge2Sb2Te5 — •Julian Pries[1], Shuai Wei[1], Matthias Wuttig[1,2], and Pierre Lucas[3] — [1]Institute of Physics IA, RWTH Aachen University, Germany — [2]Peter Grünberg Institute (PGI 10), Forschungszentrum Jülich, Germany — [3]Department of Materials Science and Engineering, University of Arizona, United States

Phase-Change materials (PCMs) can be switched in nanoseconds between the amorphous and crystalline phase. In combination with the pronounced change of physical properties like electrical resistivity or optical reflectivity upon this transition, PCMs offer a wide potential for memory applications. A deep understanding of crystallization kinetics is essential for increasing the data transfer rate of such devices. Here,

crystallization kinetics of the prototypical PCM Ge2Sb2Te5 is investigated. Combining conventional and Flash DSC opens a heating rate interval of over six orders of magnitude. The resulting crystallization data reveals a sharp transition from a high to a low Kissinger activation energy of crystallization when exceeding the critical heating rate. Moreover, pre-annealing affects this activation energy at low, but not at high rates. Utilizing Fluctuation Electron Microscopy and JMAK-simulations uncovers the origin of this behavior: The manifestation of glass dynamics and glass transition in crystallization behavior. Accordingly, Ge2Sb2Te5 crystallizes from the glass at low and undercooled liquid phase at high heating rates. The presence of this transition has major consequences for estimating the performance of PCM memory.

MM 36.3   Thu 10:45   H46

Crystallization behavior of a bulk metallic glass-former — •Mark Stringe, Joachim Bokeloh, Harald Rösner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, D-48149 Münster

Crystallization plays a crucial role not only regarding the production of metallic glasses, but also concerning the stability of these systems. This stability is linked to the corresponding ability of atoms to rearrange. The movement of atoms is also affecting the glass forming ability and thus the crystallization of the undercooled liquid.

With a variation of scanning rates of calorimetric measurements it is possible to analyze crystallization kinetics. The measurements are performed with conventional differential scanning calorimetry (DSC). Higher scanning rates are realized using a custom-built fast DSC according to the concept of C. Schick et al. [1]. With this fast scanning calorimetry (FSC) samples with a mass of the order of micrograms are measured with scanning rates up to 10.000 K/s.

An AuCuSiAg bulk metallic glass with low melting point is analyzed. In FSC it is possible to reach cooling rates to quench a glass in-situ. Thus the critical cooling rate can be determined directly and activation energies for crystallization of the supercooled liquid are obtained from Kissinger analyses.

Depending on the degree of undercooling, the system shows a change in the crystallization behavior of the undercooled liquid suggesting a change in kinetics.

[1] Zhuravlev E, Schick C, Thermochimica Acta 505 (2010) 1-13

MM 36.4 Thu 11:00 H46

Quasi-discontinuous change of the density correlation length at the fragile-to-strong transition in a bulk-metallic-glass forming melt — •Sergey V. Sukhomlinov and Martin H. Mueser — Universität des Saarlandes, 66123 Saarbrücken, Germany

Many bulk-metallic-glass (BMG) forming melts undergo a fragile-to-strong transition (FST), which is accompanied by a small but noticeable peak in the specific heat c_p. However, density and local structure at the FST appear to change only continuously. Because of the peak in the c_p, the FST is sometimes interpreted as a smeared-out phase transition. This motivated us to study how the specific heat, dynamical and structural properties of a selected BMG depend near the FST temperature on the system size using computer simulations.

For a ternary BMG former ($Zr_{0.606}Cu_{0.29}Al_{0.104}$), in contrast to the expectations for a phase transformation, we observed that the larger the system the smaller the peak in c_p. This result, along with size dependence of other properties, is difficult to reconcile with the interpretation of the FST being a (smeared-out) phase transformation.

The results from structural analysis showed a smooth evolution of radial distribution functions (RDF) at small distances through the FST. However, the long-range density correlation length increases (quasi-) discontinuously at the FST as revealed by an Ornstein-Zernike-based analysis of the RDF. Likewise, the temperature derivative of the Zr-Zr mean nearest-neighbor distance decreases (quasi-) discontinuously at the FST. These observations add to the rich phenomenology of FSTs lacking a theoretical understanding.

MM 36.5 Thu 11:15 H46

Effect of Co microalloying on thermodynamic and kinetic properties of a $Pd_{40}Ni_{40}P_{20}$ bulk metallic glass — •René Hubek[1], Mikhail Seleznev[2], Isabelle Binkowski[1], Martin Peterlechner[1], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Germany — [2]Togliatty State University, Togliatty, Russia

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

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

15 min. break

MM 36.6 Thu 11:45 H46

Origin of Large Plasticity in Fe50Ni30P13C7 Bulk Metallic Glass — •Baran Sarac[1], Yurii P. Ivanov[2], Mihai Stoica[3], and Jürgen Eckert[1,4] — [1]Erich Schmid Institute of Materials Science, Leoben, Austria — [2]University of Cambridge, Cambridge UK — [3]ETH Zurich, Zurich, Switzerland — [4]Montanuniversität Leoben, Leoben, Austria

Despite Fe-based bulk metallic glasses (BMGs) garner great interest owing to their combined high temperature thermal stability, soft magnetic properties along with high strength, the biggest barrier against a more widespread use is their negligible plasticity. A newly developed Fe50Ni30P13C7 BMG overcome this limitation via extensive compressive plasticity [1]. Using a combination of an aberration-corrected high-resolution transmission electron microscopy (HRTEM) and nanoindentation techniques, we identified a multi-stage deformation mechanism involving 1-1.5 nm sized homogeneously dispersed crystals and microscale heterogeneities [2]. Besides, we conducted a systematic set of simulations of the HRTEM images at varying sample thicknesses, and adopted a cooperative shearing model for the estimation of the shear transformation zone size of Fe50Ni30P13C7 BMG. The findings in-

dicate that the controlled nanocrystal-induced plasticity with crystal sizes of several nanometers contributes to the remarkable shear observed under quasi-static compression and enhance the plasticity of the BMG through the initiation and impediment of STZs. [1] W.M. Yang et al., Sci Rep, 4, 6233 (2014) [2] B. Sarac, et al., Nat Commun, 9, 1333 (2018)

MM 36.7 Thu 12:00 H46

Dr — •Alexandra E. Lagogianni, Muhammad Hassani, and Fathollah Varnik — ICAMS, Ruhr-Universitaet Bochum

Probing the degree of heterogeneity within the shear band of a model glass Alexandra E. Lagogianni, Muhammad Hassani and Fathollah Varnik 1ICAMS, Ruhr-Universität Bochum, Universitätsstraße 150, 44780 Bochum, Germany

We employ large scale molecular dynamic simulations to study the degree of heterogeneity within the shear band of a model sheared glass in the athermal limit. The heterogeneity, demonstrated as spatial variations of microscopic quantities such as density, local strain and viscosity, is tracked along the propagation direction of the shear band. The spatial evolution of these quantities inside the shear band shows a position-dependent nature and a sinusoidal-like pattern with a large characteristic length scale. By probing the correlations of the quantities at the stationary plastic region, we provide a quantitative analysis of the underlying mechanism and the local environment of the shear band. These correlations, captured by a simple glass forming model, are suggested to be a generic feature of metallic glasses rather than material-specific properties.

MM 36.8 Thu 12:15 H46

Size-dependent failure of the strongest bulk metallic glass — •Ruitao Qu[1,2], Dominik Tönnies[1], Lin Tian[1], Zengqian Liu[2], Zhefeng Zhang[2], and Cynthia Volkert[1] — [1]Institute of Materials Physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang, 110016, China

Upon reducing sample size into the sub-micrometer scale, the mechanical behavior of metallic glasses (MGs) is often changed dramatically. For instance, obvious tensile ductility and necking can be observed in nano-scale MGs, while they are rarely seen in bulk samples. Here we present our recent studies on the size effect of the deformation and failure behaviour of a Co-based MG, which exhibits the highest strength among all known bulk MGs. An obvious brittle-to-ductile transition accompanied by a drastic change of failure mode were observed on decreasing the sample size. The bulk compressive samples failed by splitting and shattering, similar to other brittle MGs, while the micrometer and sub-micrometer scale specimens demonstrated shear banding, typical of ductile MGs. In order to assess whether this size effect was caused by the reduced probability of the presence of defects in small-scale samples, we intentionally designed various micropillar specimens containing defects. However, no brittle failure was observed in the defective micropillars, even though the local maximum tensile stress in front of defects had far exceeded the critical tensile stress for splitting in bulk sample. A characteristic distance model for cleavage cracking initiation in brittle MGs is proposed to explain these observations.

MM 36.9 Thu 12:30 H46

Design of thin film metallic glasses with superior fracture toughness — •Simon Evertz[1], Ines Kirchlechner[2], Rafael Soler[2], Christoph Kirchlechner[2], Paraskevas Kontis[2], Volker Schnabel[3], Gerhard Dehm[2], Dierk Raabe[2], and Jochen M. Schneider[1] — [1]Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, 52074 Aachen, Germany — [2]Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany — [3]Laboratory for Nanometallurgy, ETH Zürich, Vladimir-Prelog-Weg 5, 8093 Zurich, Switzerland

Damage tolerance, i.e. the combination of high yield strength and fracture toughness, is crucial for the application of metallic glasses as structural materials. One fingerprint for damage tolerance in metallic glasses is the fraction of hybridized bonds (Schnabel et al., Scientific Reports 6 (2016) 36556), which is affected by alloying $Pd_{57.4}Al_{23.5}Y_{7.8}M_{11.3}$ with M = Fe, Co, Ni, Cu, Os, Ir, Pt and Au. Based on these ab initio calculations, the minimum fracture toughness was identified for $Pd_{57.4}Al_{23.5}Y_{7.8}Ni_{11.3}$. Furthermore, it is shown that by correlating experimental fracture toughness data to the fraction of hybridized bonds scaling with the crystal orbital overlap population at the Fermi level, the fracture toughness can be estimated based on electronic structure data. The fracture toughness

of $Pd_{57.4}Al_{23.5}Y_{7.8}Ni_{11.3}$ is predicted to be in the range of 90 to 150 $MPa.m^{0.5}$ exhibiting a plastic zone size of 0.1 to 1 mm, which is consistent with micro-mechanical beam bending experiments, where fracture was not observed.

MM 36.10   Thu 12:45   H46
Atomic-scale deformation in metallic glass nanolaminates with shape memory alloys — •Daniel Şopu[1,2], Karsten Albe[1], and Jürgen Eckert[2,3] — [1]Technische Universität Darmstadt, Otto-Berndt-Straße 3, D-64287 Darmstadt, Germany — [2]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, A-8700 Leoben, Austria — [3]Department Materials Physics, Montanuniversität Leoben, Jahnstraße 12, A-8700, Leoben, Austria

Crystalline-metallic glass laminates with shape memory alloys represent a class of material with enhanced mechanical performance superior to those predicted from a simple rule-of-mixtures. Here, we model the deformation behavior of metallic amorphous Cu64Zr36/crystalline B2 CuZr nanolaminate systems using molecular-dynamics computer simulations. First, a modeling strategy is developed to capture the autocatalytic chain-type deformation mechanism. We find that the deformation of the glassy and crystalline phases is a coupled process: martensitic transformation leads to shear band formation while the stress at the shear band tip induces martensitic transformation in the shape memory crystal. Moreover, the martensitic transformation changes the shear band morphology, stabilizes the shear flow and avoids a runaway instability. Finally, we differentiate the contributions of the aspect ratio, laminate thickness, volume fraction and structural rejuvenation to the plasticity. Therefore, tailoring the architecture of metallic glass laminates with shape memory phases may allow the development of materials that exhibit large tensile ductility.

MM 37: Topical session (Symposium MM): Big Data Analytics in Materials Science

Sessions: Big Data Analytics in Materials Science III and IV

Time: Thursday 15:00–18:45   Location: H43

Topical Talk   **MM 37.1   Thu 15:00   H43**
Atomistic Machine Learning between Physics and Data — •Michele Ceriotti — EPFL, Lausanne, Switzerland

Statistical regression techniques have become very fashionable as a tool to predict the properties of systems at the atomic scale, sidestepping much of the computational cost of first-principles simulations and making it possible to perform simulations that require thorough statistical sampling without compromising on the accuracy of the electronic structure model. In this talk I will argue how data-driven modelling can be rooted in a mathematically rigorous and physically-motivated framework, and how this is beneficial to the accuracy and the transferability of the model. I will also highlight how machine learning - despite amounting essentially to data interpolation - can provide important physical insights on the behavior of complex systems, on the synthesizability and on the structure-property relations of materials. I will give examples concerning all sorts of atomistic systems, from semiconductors to molecular crystals, and properties as diverse as drug-protein interactions, dielectric response of aqueous systems and NMR chemical shielding in the solid state.

MM 37.2   Thu 15:30   H43
Atomic cluster expansion for accurate and transferable interatomic potentials — •Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

The atomic cluster expansion provides a complete descriptor of the local atomic environment. The effort for evaluating the atomic cluster expansion scales linearly with the number of neighbors, irrespective of the order of the expansion. This makes the atomic cluster expansion an attractive basis for the development of accurate and transferable interatomic potentials.

I will discuss the application of the atomic cluster expansion to small Cu clusters and demonstrate smooth convergence to meV accuracy. I will further show how an interatomic potential that is transferable from free atoms to bulk may be obtained by combining the atomic cluster expansion with classical interatomic potentials.

MM 37.3   Thu 15:45   H43
Simultaneous and Reinforced Learning of Materials Properties from Incomplete Databases with Multi-Task SISSO — •Emre Ahmetcik, Runhai Ouyang, Christian Carbogno, Matthias Scheffler, and Luca M. Ghiringhelli — Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin-Dahlem, Germany

Identifying descriptors that capture the underlying mechanisms for different materials properties is a key challenge in data-driven materials science. Recently, the sure-independence screening and sparsifying operator (SISSO) [1] has been introduced and was successfully applied to a number of key materials-science problems [1-3]. SISSO is a compressed-sensing based methodology yielding predictive and insightful models identified from an enormous space (billions or more) of candidate analytical expressions. In this work, we have extended the methodology to a 'multi-task learning' approach, a powerful and nontrivial generalization which identifies a single descriptor capturing multiple target materials properties at the same time. This approach is specifically suited for a heterogeneous materials database with missing data, i.e., in which not all properties are reported for all materials. As showcases, we address the relative stability of octet-binary compounds for several crystal phases and the metal/insulator classification of binary materials distributed over many crystal-prototype classes.

[1] R. Ouyang et. al., Phys. Rev. Mater. 2, 1-11 (2018).
[2] C. J. Bartel et. al., Nat Commun. 9, 4168 (2018).
[3] C. J. Bartel et. al., Sci. Adv., accepted (2018), arXiv:1801.07700.

MM 37.4   Thu 16:00   H43
Information-theoretic Feature Selection and its Applications in Materials Science — •Benjamin Regler, Matthias Scheffler, and Luca M. Ghiringhelli — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Feature selection is a technique for proposing subsets of relevant properties (features), along with a measure which scores the different subsets.

In this talk, we give an overview of feature selection methods applied to materials science problems and discuss how to identify relationships between fundamental properties at the atomistic scale and materials properties at the macroscopic scale. In particular, we focus on the complexity of machine-learning models and highlight the advantages of using a systematic feature selection prior to making predictions (i.e., building machine-learning models).

Moreover, we propose a parameter-free, deterministic information-theoretic feature-selection framework for identifying approximate functional relationships between properties of interest. Importantly, the framework detects redundant and irrelevant features by performing nonlinear correlation analysis.

As showcase, we apply our approach to crystal-structure and other properties prediction in a restricted class of materials such as functionalized or octet binaries.

We conclude that our approach reduces the complexity of machine-learning models, extracts the most informative set of features, and supplements the analyses and identification of relevant properties.

MM 37.5   Thu 16:15   H43
The speech of strangers in material science — •Juliana Schell[1,2], Peter Schaaf[3], Hans-Christian Hofsäss[4], and Doru C. Lupascu[2] — [1]European Organization for Nuclear Research (CERN), CH-1211 Geneva, Switzerland — [2]University of Duisburg-Essen, 45141 Essen, Germany — [3]TU Ilmenau, Gustav-Kirchhoff-Straße 5, 98693 Ilmenau, Germany — [4]Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Differently from stable nuclei, radioactive isotopes like to talk about their local environment. Human vocal communication produces sound, radioactive isotopes emit particles and photons and can act as a probe once decaying embedded in a host material. Some of them emit two consecutive gamma rays and it is convenient to find the relative probability of detecting the second photon and obtain its angular correlation in respect to the first. Humans perform many different speech acts that vary according to their intention, while the precession of the angular

correlation in time can vary with the magnetic dipole and the electric quadrupole interactions. During the past four decades, the solid-state physics programme at ISOLDE-CERN has interpreted the speech of these strangers with innovative material science research and optimized equipment. This presentation overviews the newest perturbed angular correlation results and measurement possibilities at ISOLDE-CERN [1].

[1] Juliana Schell, Peter Schaaf, and Doru C. Lupascu, Perturbed Angular Correlations at ISOLDE: a 40 years young technique, AIP Advances 7, 105017 (2017).

15 min. break

Topical Talk   **MM 37.6**   **Thu 16:45**   **H43**
High-throughput with Particle Technology — •Lutz Mädler — University of Bremen, Faculty of Production Engineering, Badgasteiner Str. 1, 28359 Bremen, Germany — Leibniz Institute for Materials Engineering IWT, Badgasteiner Str. 3, 28359 Bremen, Germany

High-throughput screening is a well-established method for scientific experimentation in chemistry and biology. Examples are heterogeneous catalysts, drug developments and nanoparticle toxicology. These methods involve the synthesis of small sample volumes often in form of particles that are quickly tested. These tests are designed to quickly obtain easily accessible data (called descriptors) that are related with a predictor function to the desired properties. The descriptor-predictor-relation is found through mathematical modelling and calibration. One particle based high-throughput concept for the evaluation of potential toxicological hazards will be presented in more detail. Furthermore, a new concept is presented which transfers high-throughput screening to the exploration of new structural metals. The method comprises the synthesis of many small alloy samples in form of particles. These samples obtain a defined microstructure by fast or parallel thermal and mechanical treatments and are subsequently subjected to novel fast descriptor tests while a mathematical algorithm develops the predictor function. The method presented here is a collaborative approach among many researchers and also involves sample routing and automation considerations, process modelling as well as big data methods.

Topical Talk   **MM 37.7**   **Thu 17:15**   **H43**
Microstructure is the know-it-all - classification approaches with data mining and deep learning methods — •Frank Mücklich[1,2] and Dominik Britz[2,1] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]Material Engineering Center Saarland, Saarbrücken, Germany

The microstructure can be regarded as the *multi-scale archive* from which we can *read* the quantitative information about the microstructure formation processes and the prediction of the final material properties on each relevant scale. Recent advances in 3D tomography methods on the micro, nano and atomic scale allow to study the differences of microstructures with higher morphological and topological complexity. Classification strategies using Support Vector Machine and Deep Learning will be discussed using morphological and substructure parameters. Images are processed directly in the workflow after an adapted contrasting. The result might be simultaneously segmented and classified.

S. M. Azimi, D. Britz, M. Engstler, M. Fritz, and F. Mücklich, Advanced Steel Microstructural Classification by Deep Learning Methods, Scientific Reports (Nature) 8 (2018) 2128.

MM 37.8   **Thu 17:45**   **H43**
Electronic density-of-states fingerprints for finding similar materials — •Martin Kuban, Santiago Rigamonti, Markus Scheidgen, and Claudia Draxl — Humboldt-Universität zu Berlin

The recent development of large databases for computational materials science, like NOMAD [1], allows researchers to reuse data that was generated for different purposes. In this work, we make use of the data contained in NOMAD to find materials with similar properties. Similarity can be evaluated and quantified by comparing specialized representations of the materials properties, so-called *fingerprints*. We design a family of fingerprints derived from the electronic density-of-states (DOS), consisting of vectorial representations obtained from non-uniform scalings of the DOS. In contrast to previous works [2], our approach allows us to set the focus of searches for similar materials on special features of the DOS, as for instance the band gap, or the amount of states close to the Fermi level. We present examples for

several materials ranging from metals to insulators. To demonstrate the usefulness and applicability of our approach, we have devised a *recommender system* for the NOMAD Encyclopedia.
[1] C. Draxl and M. Scheffler, *MRS Bulletin*, **43**, 676, (2018).
[2] O. Isayev *et al.*, *Chermistry of Materials* **27**, 735, (2015).

MM 37.9   **Thu 18:00**   **H43**
Accurate Thermal Conductivities of Complex, Strongly-Anharmonic Solids — •Florian Knoop, Thomas Purcell, Marcel Hülsberg, Matthias Scheffler, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Vibrations in modern functional materials, e.g., perovskites [1], are often governed by strongly anharmonic effects. Traditional perturbative *ab initio* approaches do not capture these effects and are thus not suited to describe the associated material properties, e.g., the lattice heat conductivity $\kappa(T)$. For these materials, $\kappa(T)$ can be accurately computed via the *ab initio* Green-Kubo (aiGK) method [2], in which anharmonic effects are fully accounted for via *ab initio* molecular dynamics (aiMD) simulations.

In our hierarchical high-throughput approach, we first compute the harmonic properties of thousands of compounds spanning over several classes of materials, including simple elemental semiconductors, but also complex technologically relevant materials such as ceramics and perovskites. From these materials, aiMD-inspired metrics are used to single out strongly anharmonic compounds, for which $\kappa(T)$ is then computed with the aiGK method. We discuss the challenges involved in this automatized approach, the reliability of our metrics, and the trends observed in materials space.
[1] A. van Roekeghem, *et al.*, *Phys. Rev. X.*, **6**, 041061 (2016)
[2] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.*, **118**, 175901 (2017).

MM 37.10   **Thu 18:15**   **H43**
Surface Structure Search using Coarse Grained Modeling and Bayesian Linear Regression — •Lukas Hörmann, Andreas Jeindl, Alexander T. Egger, and Oliver T. Hofmann — Institute of Solid State Physics, Graz University of Technology, Austria

The key information about a monolayer of molecules on a substrate, aside from chemical composition, is arguably the polymorph it forms. First-principles prediction of such polymorphs is a major challenge, due to the large number of possible arrangements of molecules. To meet this challenge, we develop SAMPLE[1,2], which uses physically motivated coarse graining and statistical learning to explore the potential energy surface of commensurate organic monolayers on inorganic substrates.

We first determine adsorption geometries of isolated molecules on the substrate. By generating commensurate arrangements of these geometries, we compile a large number of possible polymorphs. Using experimental design theory, we select subsets of these polymorphs and calculate their adsorption energies using dispersion-corrected density functional theory. These subsets serve as training data for an energy model, based on molecular interactions. Using Bayesian linear regression, we determine the model parameters, yielding meaningful physical insight and allowing the prediction of adsorption energies for millions of possible polymorphs with high accuracy.

We demonstrate this on three complimentary systems: naphthalene on Cu(111), TCNE on Cu(111), and benzoquinone on Ag(111).
[1] Hörmann et al., arXiv:1811.11702 (2018)
[2] Scherbela et al., Phys. Rev. Materials 2, 043803 (2018)

MM 37.11   **Thu 18:30**   **H43**
Predicting Reaction Energetics with Machine Learning — •Sina Stocker, Johannes T. Margraf, and Karsten Reuter — Technische Universität München, Germany

Predictive-quality first-principles based microkinetic models are increasingly used to analyze (and subsequently optimize) reaction mechanisms in heterogeneous catalysis. In full rigor such models require the knowledge of all possible elementary reaction steps and their corresponding reaction barriers. Unfortunately, for complex catalytic processes, such as the generation of synthetic fuels out of syngas, the number of such steps becomes so large that an exhaustive first-principles calculation of all barriers becomes prohibitively expensive.

As a remedy, we explore the possibility of machine learning (ML) approaches to the prediction of the reaction energetics. An essential component in such data-driven approaches are efficient molecular representations (descriptors). We test a range of such representations that have been suggested to describe properties of closed-shell molecules and

specifically assess their capabilities in describing open-shell systems and consequently reaction energetics. The obtained overall promising performance confirms the potential of ML approaches for a high throughput screening of elementary steps in large reaction networks.

MM 38: Methods in Computational Materials Modelling (methodological aspects, numerics)

Sessions: Unconventional materials; Complex alloys and microstructure

Time: Thursday 15:00–17:30   Location: H44

MM 38.1   Thu 15:00   H44
Materials with helical architecture obtained by High Pressure Torsion Extrusion — •Roman Kulagin[1], Yan Beygelzimer[1,2], Yuri Estrin[3,4], Yulia Ivanisenko[1], Dayan Nugmanov[1], Andrej Mazilkin[1,5], and Horst Hahn[1] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany — [2]Donetsk Institute for Physics and Engineering named after A.A. Galkin, National Academy of Sciences of Ukraine, Kyiv, Ukraine — [3]Department of Materials Science and Engineering, Monash University, Clayton, Australia — [4]Department of Mechanical Engineering, The University of Western Australia, Crawley, Australia — [5]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Russia

Composite materials are widely used in engineering. Commonly, reinforcements have simple shapes of granules, fibers or laminae. By using free-end torsion, one can transform straight fibers into helicoidal ones. The report describes the High Pressure Torsion Extrusion (HPTE) process, which allows performing more complex transformations. For example, straight fibers can be transformed to complex helicoidal surfaces. This greatly expands the range of achievable architectures of composites, while at the same time improving the strength of their constituents through extreme grain refinement. A simple analytical model developed in this work and verified experimentally provides a platform for design of composite materials with HPTE-induced inner architectures.

MM 38.2   Thu 15:15   H44
The Effect of the Hydrostatic Pressure on the Topology of the Electronic Charge Density of YbB_6 — •Niloofar Hadaeghi[1,2], Javad Nematollahi[1], Saeid Jalali Asadabadi[1], and Hongbin Zhang[2] — [1]Department of Physics, Faculty of Sciences, University of Isfahan, Isfahan, Iran — [2]Institute of Materials Science, Technische Universität Darmstadt, Darmstadt, Germany

Several rare-earth based hexaborides have been proposed to be strongly correlated topological Kondo insulators. In this work, the topology of the electronic charge density (TECD) for YbB_6 compound and its changes at finite pressure is investigated using density functional theory and quantum theory of the atoms in molecules, to search for possible transition in the topology of charge densities. The calculations were performed using the WIEN2k and CRITIC2 codes, within the GGA+U (U=7 eV) approximation with spin-orbit coupling. It is observed that no topological transition occurs in the charge density of YbB_6 when applying pressure, and no quasi-atom exists. Detailed analysis on the number of various types of critical points has been carried out, and the Morse relation is satisfied at both zero and finite pressures.

MM 38.3   Thu 15:30   H44
On the negative differential conductance of single-wall carbon nanotubes from ab-initio quantum simulations — •Jaime Silva[1], Bruce F. Milne[1,2], and Fernando Nogueira[1] — [1]CFisUC, Department of Physics, University of Coimbra, Rua Larga, 3004-516 Coimbra, Portugal — [2]Nano-Bio Spectroscopy Group, University of the Basque Country (UPV-EHU), Centro Joxe Mari Korta, Avenida de Tolosa, 72, 20018 Donostia-San Sebastian, Spain

Negative differential conductivity (NDC) is a current decrease when the voltage across certain materials is increased. It is important for oscillators, amplifiers, and fast switching devices. In this work, using real time quantum simulations, we show that this phenomenon occurs in isolated finite armchair single wall carbon nanotubes (SWCNT) without end contacts. For metallic SWCNT, like the armchair SWCNT, NDC due to electron transfer to secondary valleys is not expected to be observed, as a consequence of the two quantum channels at the Fermi energy that are available to conduction. The NDC is due to the finite nature of the SWCNT and the existence of excited states that

are blocked, similarly to a Coulomb blockade system, thus preventing any further current flow. We also show that the SWCNT conductivity depends on its length and that the current flowing on the SWCNT behaves like a Bloch oscillation that is disrupted in the presence of a molecule, decreasing the conductivity, which explains the behaviour of SWCNT organic gas sensors.

MM 38.4   Thu 15:45   H44
Exchange-driven dimerization, magnetism and insulating state in diamond(111) — Betul Pamuk[1] and •Matteo Calandra[2] — [1]School of Applied and Engineering Physics, Cornell University, Ithaca, NY 14853, USA — [2]Sorbonne Université, CNRS, Institut des Nanosciences de Paris, UMR7588, F-75252, Paris, France

Strong electron-electron interaction in ultraflat edge states can be responsible for correlated phases of matter, such as magnetism, charge density wave or superconductivity. Here we consider the diamond(111) surface that after Pandey reconstruction, presents zig-zag carbon chains, generating a very flat surface band. By performing full structural optimization with hybrid functionals, we find that a substantial dimerization (0.076 Å bond disproportionation in the HSE06, 0.09 Å in PBE0) occurs on the chains; a structural effect absent in calculations based on the LDA/GGA functionals. This dimerization is the primary mechanism for the opening of an insulating gap. Neglecting spin polarization, the single-particle direct gap is 1.672 in PBE0 (1.0 in HSE06), smaller than the experimental data that are compatible with a $1.57 - 1.87$ (including $0.1 - 0.4$ eV of excitonic effects). However, the exchange interaction stabilizes a ferrimagnetic order along the Pandey π-chains with magnetic moments as large as 0.285 μ_B, opening a direct band gap of approximately 2.1 eV in PBE0, in agreement with experiments. Our work is relevant for systems with flat bands in general and wherever the interplay between structural and electronic degrees of freedom is crucial, as in twisted bilayer graphene, IVB atoms on IVB(111) surfaces such as Pb/Si(111) or molecular crystals.

MM 38.5   Thu 16:00   H44
Unconventional superconductivity in a doped quantum spin Hall insulator — Xianxin Wu, Mario Fink, Werner Hanke, Ronny Thomale, and •Domenico Di Sante — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland Campus Süd, Würzburg 97074, Germany

A monolayer of jacutingaite (Pt_2HgSe_3) has recently been identified as a novel quantum spin Hall insulator. By first-principles calculations, we study its Fermiology in the doped regime and unveil a type-I and type-II van Hove singularity for hole and electron doping, respectively. We find that the common link between the propensity for a topological band gap at pristine filling and unconventional superconductivity at finite doping roots in the longer ranged hybridization integrals on the honeycomb lattice. In a combined effort of random phase approximation and functional renormalization group, we find chiral d-wave order for the type-I and odd-parity f-wave order for the type-II regime.

MM 38.6   Thu 16:15   H44
Designing new two-dimensional Janus nanomaterials by anionic exchange — •Woosun Jang[1,2] and Aloysius Soon[1] — [1]Department of Materials Science & Engineering, Yonsei University, Seoul 03722, Korea — [2]Department of Inorganic Chemistry, Fritz-Haber-Institute of the Max-Planck-Society, Berlin 14195, Germany

Two-dimensional nanomaterials have played a key role in the recent advances in nanoscience for a decade, especially in the area of energy technology. Of late, a new class of 2D material has been suggested and experimentally realized – namely, the Janus monolayer. Different from preceding 2D materials, such as graphene and transition metal dichalcogenides, Janus monolayers lack the inversion symmetry in both in-plane and out-of-plane directions, and this leads to new anisotropic physiochemical properties which can be potentially useful for key energy applications. In this work, we design and investigate various novel

two-dimensional Janus materials, via the anionic exchange method. In particular, by starting from the well-known MoS_2 and WS_2 monolayers, we substitute the top and bottom sulfur layers using a combination of group V and VII anions. Density-functional theory calculations are then performed to examine their anisotropic material properties.

15 min. break

MM 38.7 Thu 16:45 H44

Shandite Co3Sn2S2 - story and news — •RICHARD WEIHRICH — University of Augsburg, Regensburg, Germany

Shandite type compounds turned into focus with recent discoveries on Sn2Co3S2 = Co3Sn2S2 i.e. giant anomalous hall effects and magnetic Weyl semi metal characteristics. The compound was first synthesized and characterized in Regensburg in 1979 by Zabel and Range. After 2 decades the half metal ferromagnetism of highly anisotropic Sn2Co3S2 was discovered by DFT calculations in Regensburg, too. The story of the compound, discoveries and new results are reported and discussed.

MM 38.8 Thu 17:00 H44

Atomistic simulations of mixed 1/2 [111] dislocations in bcc transition metals — •TAPASWANI PRADHAN[1], ANASTASIIA KHOLTOBINA[2], LORENZ ROMANER[3], MATOUS MROVEC[4], and RALF DRAUTZ[5] — [1]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Bochum, Germany — [2]Materials Center Leoben Forschungs GmbH, Leoben, Austria — [3]MCL Forschungs GmbH, Leoben, Austria — [4]ICAMS, RUB, Bochum, Germany — [5]ICAMS, RUB, Bochum, Germany

Structure and mobility of dislocations govern the mechanical properties of metals. It is widely accepted that in body-centered cubic (BCC) metals plastic deformation at low temperature is largely controlled by non-planar $1/2<111>$ screw dislocations. However, recently mixed $1/2<111>$ dislocations, which are predominantly of edge character and therefore expected to be glissile, were proposed to possess an unexpectedly high Peierls stress. In this study we investigate the core structures and mobilities of mixed $1/2<111>$ dislocations in five BCC transition elements Nb, Ta, Mo, W and Fe using atomistic simulations. The simulations were carried out with different models of interatomic interactions, ranging from classical potentials via tight-binding-based bond order potentials to first-principles methods based on density functional theory. Our study shows that both the predicted core structures and the Peierls barriers depend sensitively on the employed model and boundary conditions. We present a detailed comparison of different models and discuss the relation between atomic-scale properties and macroscopic behavior.

MM 38.9 Thu 17:15 H44

Simulation of Capillary-Driven Kinetics with Multi-Phase-Field and Lattice-Boltzmann — •RAPHAEL SCHIEDUNG[1], MARVIN TEGLER[1], DMITRY MEDVEDEV[2], and FATHOLLAH VARNIK[1] — [1]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Bochum, Germany — [2]Lavrentyev Institute of Hydrodynamics SB RAS, Lavrentyev prosp. 15, 630090, Novosibirsk, Russia

We propose a combined computational approach based on the multi-phase-field and the lattice Boltzmann method for the motion of solid particles under the action of capillary forces. The accuracy of the method is analyzed by comparison with the analytical solutions for the force and motion of two parallel plates of finite extension connected by a capillary bridge. The method is then used to investigate the dynamics of multiple spherical solid bodies connected via capillary bridges. The amount of liquid connecting the spheres is varied, and the influence of the resulting liquid-morphology on their dynamics is investigated. It is shown that the method is suitable for a study of liquid-phase sintering which includes both phase transformation and capillary driven rigid body motion [1]. Furthermore, the combination with the multi-phase-field offeres the possibility to include effects relevant to solid-phase sintering [2, 3].

MM 39: Structural Materials (Steels, light-weight materials, high-temperature materials)

Sessions: Advanced steels; High temperature compounds

Time: Thursday 15:00–17:45   Location: H45

MM 39.1 Thu 15:00 H45

Impact of Ferritic, Pearlite and Martensitic Micro-structured Steels and Geometric Length Scales on Micro Tensile Testing — •JONAS KUTSCHMANN[1,2], THOMAS PRETORIUS[2], ANDREAS OFFERGELD[2], ANDREAS KERN[2], and GERHARD WILDE[1] — [1]Institute of Materials Physics, Westfälischen Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster — [2]thyssenkrupp Steel Europe AG, Kaiser-Wilhelm-Straße 100, D-47166 Duisburg

Mechanical properties of different microstructures of steels are characterized by micro tensile tests and compared to other mechanical testing methods. Out of the heavy plates, provided by thyssenkrupp, miniaturized specimens with a dog-bone shape contour were cut. The specimen dimensions are of constant gauge length of 4 mm, with a gauge width between 0.3 mm and 0.5 mm and a gauge thicknesses between 1.5 mm and 0.05 mm. The depth profile of the heavy plates are correlated to mechanical properties. The thickness of the specimens has been varied over a considerable range to verify an occurring specimen size effect.

The tensile test results are correlated to Vickers hardness measurements, average grain sizes by EBSD and macro tensile tests for the ultimate tensile strength. All steels show a linear correlation between Vickers hardness and tensile strength. Micro testing of the steels reproduce the macro-scale results well. The tensile strength is almost unaffected by down-scaling of the thickness for small grain sizes. In contrast, the fracture strain decreases together with decreasing dimension.

MM 39.2 Thu 15:15 H45

High Temperature Chlorine Corrosion - Influence of additives on alkali-capture and the effect on corrosion in waste to energy plants — •SEBASTIAN PENTZ[1], DANIEL OTT[1], FERDINAND HAIDER[1], and RAGNAR WARNECKE[2] — [1]Universität Augsburg, Institut für Physik, 86159 Augsburg — [2]Gemeinschaftskraftwerk Schweinfurt GmbH, 97424 Schweinfurt

High temperature corrosion especially in waste-to-energy-plants leads to massive problems. At prevalent temperatures around $400°C$-$600°C$ corrosion is mainly chlorine induced. Responsible for the supply of chlorine at heat exchangers like superheaters or boiler walls is in majority a local release of chlorine through sulfation of solid alkali chlorides out of deposits on the steel parts. This reaction requires an atmosphere containing SO_2, H_2O, O_2 and releases HCl/Cl_2. Due to additive addition in the incinerator one tries to minimize this deposit built up. While encapturing alkalies by additives the formation of alkali chlorides is reduced which leads to less condensation of gaseous alkali chlorides on colder steel parts and therefore a reduction of chlorine enriched deposits. One possible material class for alkali-capture seem to be aluminum silicates. The interstratification of alkalies out of alkali chlorides into aluminium silicates leads to a release of chlorine. The corrosive attack of the steel through chlorine strongly depends on the released chlorine species. HCl is much less critical than Cl_2. Principles of the reaction conditions in waste-to-energy-plants are shown and laboratory experiments regarding the additive influence on kinetics of sulfation reactions and the corresponding chlorine attack are presented.

MM 39.3 Thu 15:30 H45

Theoretical modeling of interstitial carbon impurities in Fe-Mn paramagnetic alloys — ALENA PONOMAREVA[1], BOBUR MUKHAMEDOV[1], and •IGOR ABRIKOSOV[1,2] — [1]Materials Modeling and Development Laboratory, National University of Science and Technology "MISIS", 119049 Moscow, Russia — [2]Department of Physics, Chemistry, and Biology (IFM), Linköpings University, SE-58183 Linköping, Sweden,

We present a generalization of a model that takes into account the magnetic disorder of paramagnetic host with interstitial point defects [1] towards the case of the alloys. In the framework of disordered local

moment picture combined with magnetic sampling method, we calculate a solution enthalpy of carbon impurity in the paramagnetic fcc Fe-Mn steels. First, we use the magnetic special quasirandom structure (M-SQS) method for simulation of the paramagnetic state in Fe-Mn alloys without impurity. Here, Fe and Mn atoms are randomly distributed at the sites of a supercell. Next, to calculate the energies for various magnetic realizations around the interstitial carbon impurity, we move the position of the impurity within the SQS. Our calculations show that in alloys containing about 20 at. % Mn, the solution enthalpy of carbon reduces compared to the pure fcc-Fe. By analyzing the local and global effects of impurity on the properties of the matrix, we discuss various factors that could increase the carbon solubility in high-manganese austenitic steels.

[1] A. V. Ponomareva, Yu. N. Gornostyrev, and I. A. Abrikosov, Phys. Rev. B 90, 014439 (2014).

MM 39.4   Thu 15:45   H45
Quantum-mechanical study of thermodynamic and magnetic properties of disordered Fe-Al phases with vacancies —
•Ivana Miháliková[1,2], Martin Friák[1,2], David Holec[3], Nikola Koutná[1,2,4], and Mojmír Šob[5,1,6] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Brno, Czech Republic — [3]Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Leoben, Austria — [4]Institute of Materials Science and Technology, TU Wien, Vienna, Austria — [5]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [6]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

Iron aluminides have a great potential to substitute stainless steels in high temperature applications because of excellent chemical resistance to corrosion, reasonable strength and low material cost. We perform quantum-mechanical calculations to examine the thermodynamic and magnetic properties of disordered α-phase Fe-18.75 at.%Al with vacancies, using density functional (DFT). In order to reveal the relations between magnetic and structural properties of the α-phase on one hand and the distribution of atoms on the other, three different models of special quasi-random structure (SQS) were used. The properties of phases and, in particular, local magnetic moments of the Fe atoms are found to sensitively depend on the number of Al atoms in the 1st and 2nd nearest neighbor shell of Fe atoms.

45 min. break

MM 39.5   Thu 16:45   H45
Atomic force microscopy based electrical characterization of multiphase intermetallic TiAl alloys — •Markus
Kratzer[1], Michael Huszar[1], Lisa Tengg[2], Helmut Clemens[2], Svea Mayer[2] und Christian Teichert[1] — [1]Institute of Physics, Montanuniversitaet Leoben, 8700 Leoben, Austria — [2]Department of Physical Metallurgy and Materials Testing, Montanuniversitaet Leoben, 8700 Leoben, Austria

Atomic force microscopy - a powerful tool for the characterization of surface morphologies on the meso- and nanoscale - is also applicable for the investigation of local microscale electrical properties. This is demonstrated for an intermetallic TiAl alloy. Due to their high creep resistance, low density, and high specific strength TiAl alloys are promising materials for high-temperature structural parts in advanced propulsion systems. However, besides the mechanical parameters also the electrical behaviour of the alloys and its constituting phases are of importance. For example, the electrical homogeneity of the material is of interest for the proper interpretation of the results form electrical test procedures like, e.g., eddy current testing. TiAl samples comprising three different crystallographic phases were investigated utilizing Conductive Atomic Force Microscopy (C-AFM) to reveal local conductivity variations on the surface. Complementary, local differences in the work function were mapped using Kelvin Probe Force Microscopy (KPFM). Local current-to-voltage characteristics of the existing micrometer sized phases, recorded by C-AFM, indicated significant differences in the electrical conductivity between the individual phases.

MM 39.6   Thu 17:00   H45

MM 39.6   Thu 17:00   H45
Magneto-crystalline anisotropy and magnetostriction of $\mathbf{Fe_2Ti}$ —
•Agnieszka L. Kozub[1,2], Alexander B. Shick[2], and Dominik Legut[3] — [1]Universität Paderborn, Paderborn, Germany — [2]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [3]IT4Innovations National Supercomputing Center VSB - Technical University Ostrava, Ostrava, Czech Republic

In comparison to the classical ferromagnets, the studies of magnetostriction of antiferromagnets are limited and gained recent attention. In this work we present a theoretical study of magnetic properties of Fe_2Ti, an antiferromagnet which crystallize in hexagonal C14 Laves phase. Calculations were performed in the framework of the density functional theory using generalized gradient approximation. We focus on magnetic properties of the compound, i.e. to determine its magnetic structure, and to compute magneto-crystalline anisotropy. From the magnetic anisotropy dependence of the lattice strain we estimate magnetostrictive coefficients. Finally, we investigate the effect of under- and over- stoichiometric composition of $Fe_{100-x}Ti_x$ on the magnetostriction.

MM 39.7   Thu 17:15   H45
A quantum-mechanical study of thermodynamic and mechanical stability of Heusler-based $\mathbf{Fe_2AlCo}$ **polymorphs** —
•Martin Friák[1], Sabina Oweisová[1,2], Jana Pavlů[3,2,1], David Holec[4], and Mojmír Šob[2,1,3] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic — [3]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [4]Department of Materials Science, Montanuniversität Leoben, Leoben, Austria

We use quantum-mechanical calculations to test a hypothesis of Grover *et al.* (J. Mag. Mag. Mater. 15 (1980) 699) that Co atoms in the Fe_2AlCo compound have on average 3 Fe and 3 Co atoms in their second nearest neighbor shell. We have simulated four structural configurations of Fe_2AlCo including the full Heusler structure, inverse Heusler polymorph and two phases matching this idea. The highest thermodynamic stability at T = 0 K is indeed predicted for one of the phases with the distribution of atoms according to Grover and co-workers. However, small energy differences among three of the studied polymorphs lead to a disordered B2-like phase at elevated temperatures. The fourth variant, the full Heusler phase, is predicted to be mechanically unstable. All studied variants are predicted to be ferromagnetic but local magnetic moments of Fe and Co atoms sensitively depend on the composition of the first and second coordination shells. For details see Materials 11 (2018) 1543, doi: 10.3390/ma11091543.

MM 39.8   Thu 17:30   H45
The surface and interface structures in nanofiber-reinforced ceramic matrix composites —
•Yanhui Zhang and Stefano Sanvito — School of Physics and CRANN, Trinity College Dublin, Dublin, Ireland

Surfaces and interfaces are active sites for chemical reactions, stress/strain concentration and defect accumulation. Efficiently engineering them is critical for the R&D of novel composites in the industry sectors of aerospace, automotive and energy & power. Interfacial parameters are often inaccessible by experimental measurements due to the nano-scale of interface regions. Given the importance of surface morphology on the interface adhesion and mechanical responses, we firstly examine by first-principles thermodynamics the stable surfaces of the promising ceramic matrix materials TiB2, ZrB2 and HfB2. Thereafter, we took at one specific ceramic matrix composite, namely graphene-reinforced ZrB2, to systematically explore the structural, energetic and mechanical characters of heterophase interfaces. We demonstrate that the surface chemistry of the ZrB2 matrix material largely shapes the interface structures (Zr-C-Zr or B-C-B) and the nature of the interfacial interactions. Interestingly, the mechanical responses of strong Zr-C-Zr interfaces are significantly influenced by the corrugation of graphene; while the B-C-B interfaces with relatively weak pi-pi stacking show similar attributes as the 2D materials during interfacial cleavage and slip. Those results provide insights into the interface bonding mechanisms in graphene/ceramic composites, and emphasize the prospect of interface engineering via surface chemistry.

MM 40: Liquid and Amorphous Metals

Session: Relaxation, ageing and rejuvenation

Time: Thursday 15:00–16:15   Location: H46

MM 40.1   Thu 15:00   H46

Long-range strain correlations in 3D quiescent glass forming liquids — •Muhammad Hassani and Fathollah Varnik — ICAMS, Ruhr-Universität Bochum, 44801, Bochum, Germany

Recent 2D computer simulations and experiments indicate that supercooled liquids and glasses exhibit long-lived, long-ranged strain correlations in the unperturbed quiescent state [1, 2]. Here we investigate this issue in three dimensions via molecular dynamics simulations of a glass forming binary Lennard Jones mixture. Both in the glassy state and in the supercooled regime, strain correlations are found to decay with a $1/r^3$ power-law behavior, reminiscent of elastic field around an inclusion. Moreover, theoretical predictions on the time dependence of the correlation amplitude are in line with the results obtained from simulations. It is argued that the size of the domain, which exhibits a "solid-like" strain pattern in a supercooled liquid, is determined by the product of the speed of sound with the structural relation time. While this length is of the order of nanometers in the normal liquid state, it grows to macroscale when approaching the glass transition [3, 4].

[1] B. Illing, S. Fritschi, D. Hajnal, C. Klix, P. Keim, and M. Fuchs, Phys. Rev. Lett. 117, 208002 (2016).
[2] K.E. Jensen, D.A. Weitz and F. Spaepen, Phys. Rev. E 90, 042305, (2014).
[3] M. Hassani, P. Engels, and F. Varnik, Europhys. Lett., 121(1):18005, (2018).
[4] M. Hassani, E. M. Zirdehi, K. Kok, P. Schall, M. Fuchs, and F. Varnik, Europhys. Lett., 124(1):18003, (2018).

MM 40.2   Thu 15:15   H46

The relaxation dynamics of a severely deformed metallic glass studied by X-ray photon correlation spectroscopy — •Hongbo Zhou[1], Sven Hilke[1], Eloi Pineda[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, 10 Wilhelm-Klemm Strasse, Münster 48149, Germany — [2]Department of Physics, Universitat Politecnica de Catalunya BarcelonaTech, Esteve Terradas 8, Castelldefels 08860, Spain

The structural relaxation behavior of a metallic glass severely deformed by High- Pressure Torsion was investigated at the atomic length scale by high-resolution X-ray photon correlation spectroscopy. We find that the dynamics of the deformed sample is much faster compared with the undeformed sample, indicating that rejuvenation has occurred. Meanwhile, the structural relaxation rates and behaviors of both samples are distinct at different temperatures. It is notable that an intermittent and heterogeneous relaxation process happens at the temperature of 423 K. The activation energies of the structural relaxation below 473 K are 21.2 kJ/mol and 25 kJ/mol respectively, which demonstrates that the relaxation processes at low temperatures are stress-dominated. However, when the temperature is increased above 473 K, a crossover behavior of the effective relaxation time occurs, which is probably due to a change of relaxation mechanisms from a stress-dominated to a diffusion-dominated process.

MM 40.3   Thu 15:30   H46

Characterization of CuZr-based bulk metallic glasses rejuvenated by severe plastic deformation — Christian Ebner[1], Benjamin Escher[2], Christoph Gammer[3], Jürgen Eckert[3], Simon Pauly[2], and •Christian Rentenberger[1] — [1]University of Vienna, Physics of Nanostructured Materials, Vienna, Austria — [2]Leibniz Institute for Solid State and Materials Research Dresden, Institute for Complex Materials, Dresden, Germany — [3]Austrian Academy of Sciences, Erich Schmid Institute of Materials Science, Leoben, Austria

Bulk metallic glasses (BMGs) are materials composed of metal components but lack long-range order. The latter renders BMGs unique in their mechanical properties. Nevertheless, they exhibit also a low ductility caused by a very localized plastic deformation. Therefore, it is one of the challenging aims to find ways and processes for improvements. In this work we show that severe plastic deformation of BMGs facilitates a rejuvenation of the disordered atomic structure that was characterized by various methods including Synchrotron X-ray diffraction, nanoindentation, differential scanning calorimetry, atomic force and transmission electron microscopy. By a unique and unprecedented mapping of structural and mechanical quantities on micrometer scale a clear correlation both between elastic and plastic softening and between softening and mean atomic volume can be revealed [1]. Finally, based on nanoindentation curves it is concluded that structural rejuvenation promotes a more homogeneous like deformation.

[1] C. Ebner et al., Acta Mater 160 (2018) 147.
Support by the Austrian Science Fund FWF: I1309 is acknowledged.

MM 40.4   Thu 15:45   H46

Impact of cryogenic rejuvenation on calorimetric and kinetic properties of plastically deformed $Pd_{40}Ni_{40}P_{20}$ bulk metallic glass — •Afrouz Hassanpour, Sergiy V. Divinski, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics University of Münster Wilhelm-Klemm-Str. 10 48149 Münster Germany

In metallic glasses, plastic deformation at ambient conditions is typically localized in shear bands. In the present work, the impact of different types of deformation, namely of high-pressure torsion (HPT) and cold rolling, and the effect of subsequent cryogenic rejuvenation are analyzed for the $Pd_{40}Ni_{40}P_{20}$ bulk metallic glass. Different experimental techniques are applied to examine the structural changes due to the plastic flow, including X-ray diffraction, differential scanning calorimetry and the radiotracer diffusion measurement. Using HPT processing, extremely large shear deformation is imposed under quasi-hydrostatic conditions. The plastic flow during deformation likely increases the excess free volume in the material and affects the local atomic configurations. We report on an increase of the diffusion rates in the deformed samples in comparison to the as-cast ones and the impact of cryogenic rejuvenation on the diffusion enhancement. Shear bands are shown to represent short-circuit paths for diffusion and their relaxation is discussed.

MM 40.5   Thu 16:00   H46

Decelerated Ageing in Binary Metallic Glasses by Cryogenic Thermal Cycling — •Marian Bruns and Fathollah Varnik — Ruhr Universität Bochum, Universitätsstraße 150, 44801 Bochum, Germany

Cryogenic thermal cycling is a thermal treatment where samples are exposed to an oscillatory temperature change at low temperatures. For its application to metallic glasses, cycling temperatures sufficiently below the glass transition temperature T_G are employed to avoid thermally activated relaxation or annealing. It has been proposed that cryogenic thermal cycling leads to rejuvenation of aged glasses, thus improving their plasticity.

Here, we investigate this issue via molecular dynamics simulations. In contrast to previous studies, addressing static properties, we focus on dynamic aspects. We qualitatively indicate ageing, rejuvenation and their extend by comparing the *mean squared displacement* of as-aged and as-cycled systems. The treatment has been performed at both constant volume and constant pressure with different frequencies, depending on the time the system aged prior to the cycling. We find that the glassy system as we prepared it is not being rejuvenated by the treatment but further ageing during the cycling is observable. Nonetheless the treatment has an impact on the ageing process by slowing it remarkably down. This indicates that processes that cause ageing (i.e. structural relaxation) are in a competitive relation with processes related to rejuvenation due to thermal treatment.