MM 29: Poster II

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

MM 29.1 Tue 17:00 Poster B

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

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

MM 29.2 Tue 17:00 Poster B

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

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

MM 29.3 Tue 17:00 Poster B

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

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

MM 29.4 Tue 17:00 Poster B

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

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

MM 29.5 Tue 17:00 Poster B

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

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

MM 29.6 Tue 17:00 Poster B

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

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

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

MM 29.7 Tue 17:00 Poster B

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

Resonant Inclastic X-ray Scattering (RIXS) provides element specific information on both occupied and unoccupied states, and on two-

particle excitations of the material. This spectroscopy technique correlates the emitted photons with the incident X-ray photons. Recent improvements in synchrotron radiation sources provide an energy resolution which allows for a detailed comparison with calculated spectra. In view of ongoing experimental investigations related to the oxygen evolution reaction in manganites we performed ab-initio first-principles calculations to explore the correlation of RIXS spectra with chemical processes.

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

MM 29.8 Tue 17:00 Poster B

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

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

MM 29.9 Tue 17:00 Poster B

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

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

MM 29.10 Tue 17:00 Poster B

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

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

MM 29.11 Tue 17:00 Poster B

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

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

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

MM 29.12 Tue 17:00 Poster B

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

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

MM 29.13 Tue 17:00 Poster B

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

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

MM 29.14 Tue 17:00 Poster B

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

neering, Mugla University

Five or six-component high entropy alloys have been known in materials research for a long time and stand out due to their good mechanical properties [1]. CrMnFeCoNi, which has the same electronic configuration as fcc-Fe with an electron per atom ratio of e/a = 8, plays a crucial role here. Increasing the lattice constant in fcc-Fe changes the magnetic ordering from antiferromagnetic to ferromagnetic, which is also valid for CrMnFeCoNi [2]. Introducing interstitial carbon leads to a lattice expansion up to 0.02 Å [2]. Besides interstitial C, B can also be used to expand the volume of the lattice. Here, we investigate the effect of increasing interstitial C and B content on the structural and magnetic ordering by the combination of SEM, EDX, Mössbauer spectroscopy, XRD and magnetometry.
We acknowledge the financial support through the Deutsche Forschungsgemeinschaft wihtin the framework of the CRC/TRR270 HoMMage (Project 405553726-TRR270).

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

MM 29.15 Tue 17:00 Poster B

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

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

MM 29.16 Tue 17:00 Poster B

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

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

MM 29.17 Tue 17:00 Poster B

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

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

MM 29.18 Tue 17:00 Poster B

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

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

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

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

MM 29.19 Tue 17:00 Poster B

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

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

MM 29.20 Tue 17:00 Poster B

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

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

markedly improved conductivity. Size, shape and density of precipitates are analyzed by means of HRTEM, STEM and APT.

MM 29.21 Tue 17:00 Poster B

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

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

MM 29.22 Tue 17:00 Poster B

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

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

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

MM 29.23 Tue 17:00 Poster B

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

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

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

MM 29.24 Tue 17:00 Poster B

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

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

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

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

MM 29.25 Tue 17:00 Poster B

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

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

MM 29.26 Tue 17:00 Poster B

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

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

MM 29.27 Tue 17:00 Poster B

In-situ/ Operando Electron Microscopy Characterization of

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

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

MM 29.28 Tue 17:00 Poster B

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

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

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

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

MM 29.29 Tue 17:00 Poster B

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

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

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

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

MM 29.30 Tue 17:00 Poster B

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

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

MM 29.31 Tue 17:00 Poster B

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

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

MM 29.32 Tue 17:00 Poster B

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

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

chrotron radiation to obtain 3D time-resolved datasets of microstructural evolution and insight into the role played in AGG by second-phase particles.

MM 29.33 Tue 17:00 Poster B

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

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

MM 29.34 Tue 17:00 Poster B

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

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

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

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

MM 29.35 Tue 17:00 Poster B

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

Generating electricity in a sustainable and environmentally friendly manner is currently a topic of great concern. Thermoelectric materials, capable of directly converting heat into electricity through temperature differences, provide an effective means to harness waste heat. Doping is a practical approach to enhance thermoelectric properties, even for materials with initially poor thermoelectric performance, such as GeSe. Previous studies have demonstrated that the successful doping effects in GeSe can only be enabled by forming a metavalently bonded phase. Effective dopants such as $AgSbSe_2$ and $AgBiTe_2$ that can enable such a chemical bonding transition of GeSe from covalent to metavalent are confined in a special region of a map, where metavalently bonded compounds prevail. Yet, the universality of this concept has to be verified. Here we select PbTe from this metavalent region to alloy with GeSe. We prove that a new metavalently bonded GeSe phase can be formed with proper contents of PbTe alloying using atom probe tomography, optical property measurements, and density functional theory calculations. The resulting metavalently bonded alloy shows greatly improved thermoelectric performance by a factor of more than ten. We prove that such metavalent bonding can be a universal strategy for designing high-performance chalcogenide thermoelectrics.

MM 29.36 Tue 17:00 Poster B

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

Vacancies can be created in metals during cyclic loading, however, they have been only rarely directly detected. In this study, we develop an experimental set-up to detect fatigue generated vacancies by measuring their contribution to creep deformation. Our methodology involves performing nanoindenter creep tests on thin metal films while they are being fatigued by cyclic loading. The fatigue is realized by using delay line structures (with thin copper films on top) on which standing surface acoustic waves (SAW) are generated. Contributions from thermal drift during the creep tests have been minimized using a continuous stiffness measurement (CSM) method. The results confirm that using the developed method, it is possible to perform highly reproducible measurements. Turning the SAW loading on and off induces changes in raw displacement depth data which consistently correlate with the applied power. The CSM-corrected data also show SAW-induced changes, although not always assigned to creep behavior, but might be caused by the presence of artifacts and other effects. Initial interpretations of these variations regarding the different samples can be provided by the ellipsoidal concept of surface waves and tip asymmetry.

MM 29.37 Tue 17:00 Poster B

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

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

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

MM 29.38 Tue 17:00 Poster B

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

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