MM 30: Poster Session II

Time: Tuesday 18:15–20:00 Location: P4

MM 30.1 Tue 18:15 P4

The interplay of geometry and chemistry at Al grain boundaries: insight from atomistics — Liam Huber, •Poulami Chakraborty, Huan Zhao, Baptiste Gault, Dierk Raabe, and Joerg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf

Metallic microstructures evolve towards configurations which minimize their free energy. At the mesoscopic scale this involves the coarsening of the polycrystalline grain structure to minimize interfacial energy, but at a finer scale this interface energy can also be reduced through the formation of facets and by solute segregation. Experimental evidence from an Al-Zn-Mg-Cu alloy shows faceting of grain boundaries in this system, and a strong correlation between the grain boundary facet (i.e. geometry) and local chemistry. Using atomistic simulations, we investigate the underlying nano-scale interactions which lead to these facet-specific behaviours. A special focus is placed on the relationship between GB segregation states, which we call 'defect phases' when they are thermodynamically (meta)stable, and precipitate structure to give insight into precipitate formation in this system.

MM 30.2 Tue 18:15 P4

Resolving the grain boundary structure in nanocrystalline titanium thin films — •Vivek Devulapalli, Christian H. Liebscher, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Titanium (Ti) is an important engineering material owing to its high strength-to-weight ratio and biocompatibility. Nanocrystalline Ti (nc-Ti) can have many engineering applications making it necessary to understand the role of interfaces on material properties. However, direct atomic scale observations of GB structures in Ti are lacking and are revealed in this study using aberration corrected scanning transmission electron microscopy (STEM). In a first step, the microstructure evolution of Ti thin films obtained by different deposited techniques was investigated. Substrate temperature, ion flux and growth rate were varied to obtain textured thin films with defined tilt grain boundaries. The global film microstructure, which varied from single crystalline to nano-crystalline with different degrees of texture, were then investigated using XRD, SEM and EBSD. A nc-Ti film deposited on Si (100) contained a myriad of low angle grain boundaries and showed strong [0001] fibre texture. The atomic structure of these boundaries was further investigated by STEM. A grain boundary with 13 deg misorientation and [0001] tilt axis was composed of a dense network of [11-20] edge dislocations with a uniform spacing of 1.3nm. The intrinsic details of film growth and the resulting grain boundary structures will be discussed.

MM 30.3 Tue 18:15 P4

Observing the atomic structure of [111] tilt grain boundaries in Al — •Saba Ahmad, Christian Liebscher, and Gerhard Dehm — Max-Planck-Institute for Iron Research, 40237 Düsseldorf, Germany

Grain boundaries can be described as interface-stabilized phases which exhibit transitions between different states. These transitions are marked by discontinuous changes in grain boundary properties like mobility, cohesive strength and sliding resistance, etc. that are governed by the structure and chemistry of a grain boundary. Understanding the atomic structure of these interfacial states and the way it influences the GB properties can pave the way for GB engineering. But, a detailed understanding of the atomic structure of the GBs and their atomistic segregation behaviour is often lacking. Epitaxial aluminium thin films were deposited on (0001) sapphire substrate by electron beam evaporation technique with different deposition parameters to establish a template based methodology for obtaining specific tilt GB types. EBSD measurements were employed to characterize the global GB structure, type and fractions present in the films. Cross-sectional view TEM samples from different films were prepared using plasma (Xe) focused ion beam (FIB) to systematically study the growth of aluminium on sapphire. Also, plan-view samples having Σ13b, Σ19b, and Σ7 GBs were extracted. First results of the local atomic structure of these GBs using advanced transmission electron microscopy techniques will be reported and discussed.

MM 30.4 Tue 18:15 P4

Fractal abnormal grain growth in nanocrystalline Pd(Au): correlation between Au concentration, hardness and microstructure — •Markus Fischer[1], Raphael Zeller[1], Christian Braun[2], Jonas Endres[1], Rainer Birringer[2], and Carl E. Krill III[1] — [1]Institute of Functional Nanosystems, Ulm University, Germany — [2]Experimental Physics, Saarland University, Germany

With an average grain size below 100 nm, nanocrystalline materials often manifest enhanced mechanical properties, like higher strength or hardness, but the fine microstructure tends to go hand in hand with poor stability against grain growth. The latter generally starts at much lower temperatures than in coarser-grained specimens of the same material, and the coarsening process itself can proceed in an abnormal manner. In nanocrystalline $Pd_{90}Au_{10}$ alloys prepared by inert gas condensation (IGC), 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 ~ 1.2; this value is significantly greater than the dimension of unity for grain perimeters of conventional samples [1]. However, when Au-free nanocrystalline Pd is prepared by IGC, grain growth leads to smaller grains at impingement and smoother boundaries. To shed light on the role played by Au atoms during the coarsening of nanocrystalline Pd(Au), we have searched for correlations between grain morphology, local hardness (as revealed by nanoindentation) and the Au concentration.
[1] C. Braun *et al., Scientific Reports* **8** (2018) 1592

MM 30.5 Tue 18:15 P4

Fractal abnormal grain growth in nanocrystalline Pd(Au): a result of abnormal growth triggered by pinning centers? — •Raphael Zeller[1], Tobias Okker[1], Karina De La Torre[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 physical models have succeeded in explaining the migration of grain boundaries in polycrystals having micrometer-sized grains, our understanding of grain growth in nanocrystalline materials is still rudimentary. For example, in nanocrystalline Pd–10 at% Au produced by inert gas condensation, microstructural coarsening is found to be doubly abnormal, with a subpopulation of rapidly growing grains sending forth "tentacles" into the surrounding matrix, encircling nearby grains and then consuming them; moreover, the perimeters of the resulting grains resemble those of fractal objects. Computer simulations have ruled out two possible mechanisms for this fractal abnormal grain growth (AGG): coalescence via grain rotation and boundary migration according to highly anisotropic (reduced) mobilities. In Monte Carlo simulations reported by Holm *et al.,* pinning particles were observed to trigger explosive AGG. Since our nanocrystalline Pd–10 at% Au samples contain a small volume fraction of pores that could act as pinning centers, we performed phase field simulations to determine the pinning force per pore and to search for a connection between boundary fractality and the size and spatial distribution of pinning centers.

MM 30.6 Tue 18:15 P4

Structural relaxation in nanocrystalline Pd90Au10 — •Christian Braun, Michael J. Deckarm, Nils Boussard, and Rainer Birringer — Experimental Physics, Saarland University, Germany

The synthesis of nanocrystalline (nc) materials – either by the top-down or bottom-up approach – results in non-equilibrated material states that strongly depend on the specific sample synthesis and preparation history. Energy in excess to the crystalline ground state is stored in the disordered core regions of the interfaces as well as strain energy associated with crystal lattice distortions and the presence of lattice defects. Hence, annealing of these materials at temperatures below grain growth induces structural relaxation/aging and as a consequence the core structure of interfaces and the material properties change with time. In nc materials, structural relaxation has to be considered as a heterogeneous process due to the complex structure of the grain boundary (GB) network which can be imagined as an assemblage of structural units characterized by a site-specific deviation from local equilibrium. To adapt these heterogeneous nature of the GBs, we employed a distributed reactivity model to analyze volume relaxation of

nc Pd90Au10. This approach partitions the overall relaxation process into a set of independent and parallel reactions and was applied to a set of dilatometer data captured under different time-temperature protocols to probe the spectrum of potential barriers the material has to overcome on its way to equilibrium. Furthermore, we analyzed the corresponding change in mechanical properties and microstructure.

MM 30.7 Tue 18:15 P4

Correlative study of grain boundary segregation in nanocrystalline copper–nickel alloys — •Felix Fischer, Rüya Duran, Guido Schmitz, and Sebastian Eich — Institute for Materials Science, University of Stuttgart, Germany

Nanocrystalline material properties are dominated by grain boundaries (GB). In nanocrystalline copper–nickel alloys, which have high corrosion resistance, thermal conductivity, and fabricability, segregation of copper to GBs is energetically preferred and was previously quantified in simulations by Molecular Dynamics using a new embedded-atom alloy potential. In these simulations, the values for the solute excess depend highly on the GB structure. Comparison to experimental data is required, thus correlative transmission electron backscattering diffraction (t-EBSD) and atom probe tomography (APT) measurements are carried out on prepared nanocrystalline tips.

t-EBSD allows an evaluation of the grain orientations and thus the GB types, while APT gives an atomically-resolved digital reconstruction of the measured tip. Combing these two methods, the segregation of copper to GBs can be correlated to the GB type, alloy concentration as well as the annealing temperature and furthermore compared to the simulated segregation.

Experimental as well as simulated segregation curves will finally be compared and described by a previously developed model for interface segregation. The change in interface formation energy based on the new model will be predicted.

MM 30.8 Tue 18:15 P4

Abnormal grain growth in Al(Cu) assisted by Zener pinning — •Maria Hohm, Raphael Zeller, Mingyan Wang, and Carl E. Krill III — Institute of Functional Nanosystems, Ulm University, Germany

Abnormal grain growth occurs during the heat treatment of polycrystals when a subpopulation of crystallites undergoes rapid growth at the expense of neighboring grains, leading to a bimodal grain size distribution. In some cases, abnormal grain growth appears to be triggered by grain boundaries interacting with second-phase particles, a process called Zener pinning. Although of considerable technological importance, there is still no consensus regarding the mechanism(s) underlying abnormal grain growth assisted by Zener pinning; indeed, most experimental studies of the phenomenon have been carried out on sample sections or thin films, for which the free surface is a complicating factor. The latter limitation can be circumvented by 3D characterization techniques like diffraction-based x-ray microscopy, which are able to assess the size and morphology of grains, the lattice misorientation at grain boundaries and the distribution of pinning particles throughout a bulk specimen. From such data, we aim to identify how pinning particles initiate and govern abnormal grain growth in Al(Cu) alloys.

MM 30.9 Tue 18:15 P4

About the atomic structure of copper grain boundaries — •Lena Frommeyer, Christian H. Liebscher, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

The atomic structures of grain boundaries (GBs) as interfaces between two crystals are determining microscopic and macroscopic properties of a material. So far, GBs were mostly studied by atomistic simulations and only few experimental studies exist, investigating pure high angle GBs on an atomic level. Recent studies of pure Σ19b [111] tilt GBs in copper showed that a GB can undergo phase transformations and different atomic structures can coexist, both in symmetric and asymmetric GBs. Furthermore, two symmetric variants of the Σ19b GB were observed, having different structural units. They also show a different behavior in compensating for inclinational deviations.
In this work, the same system is used, but a different GB, the Σ37c [111] tilt GB, is analyzed. As for the Σ19b GB, two different symmetric variants are observed and their atomic structures are studied by aberration-corrected transmission electron microscopy. Furthermore, asymmetric variants are investigated to analyze their behavior in compensating for deviations from the symmetric GB plane inclination. By comparing the results to the Σ19b GB, primary conclusions can be drawn whether structural units of symmetric GBs and their asymmetric variants are unique features of specific GBs or if the relation follows a generic concept.

MM 30.10 Tue 18:15 P4

Effect of residual stresses on dislocation nucleation and motion in lamellar TiAl alloys — •Ashish Chauniyal and Rebecca Janisch — ICAMS, Ruhr Universität Bochum

Residual stresses are present within many microstructures due to lattice mismatch, curvature effects and/or processing history. These residual stresses are a known cause for microyielding and localized plasticity. In this work we study the effect of residual stresses on dislocation nucleation and motion using a two phase TiAl lamellar system. The lattice mismatch between hexagonal $\alpha_2(Ti_3Al)$,face centered tetragonal $\gamma(TiAl)$ phases creates coherency stresses in individual phases. These residual stresses are a known cause for microplasticity in lamellar TiAl. In this work we carry atomistic simulations of α_2/γ bilayers with a dislocation nucleator in γ phase which emits dislocation loops during deformation. Using this framework, we study the mechanism of emission, propagation and interface interactions of dislocations in a α_2/γ bicrystal, in correlation with coherency stresses present within the lamellae.

MM 30.11 Tue 18:15 P4

Mechanical testing of SAC soldered micro- and nanowire joints — •Samuel Griffiths and Guido Schmitz — Chair of Materials Physics, Institute for Material Science University of Stuttgart, Germany

Joining is a ubiquitous component of many modern macro- and microscopic technologies, and as such joints continue to be miniaturized, it becomes increasingly necessary to evaluate the effects of miniaturization on the mechanical properties of the structural materials. Wires are fundamental building blocks which have been extensively examined for their promising electrical/surface properties - considered for use in different micro and nano devices. Quantifications of their mechanical properties although remains limited.

Most fundamental to understanding the mechanical strengths and limitations of nanowires, is determining their dependency on diameter. Here, we present our creative methodology for mechanically testing Cu micro-/nanowires soldered to substrates with SAC to initially determine the weakest link. Additionally, our preliminary tensile results are presented in dependence of diameter. Experiments were conducted in an environmental SEM including both in-situ soldering and mechanical testing under constant temperature conditions. The phenomenological reasoning for the size dependency is also alluded to.

MM 30.12 Tue 18:15 P4

Microstructural and mechanical investigation of magnetic impulse welds of Aluminium and Copper — •David Stein[1], Maximilian Gnedel[1], Sven Winter[2], and Ferdinand Haider[1] — [1]Chair of Experimental Physics I, University of Augsburg, Universitätsstraße 1, 86159 Augsburg (Germany) — [2]Fraunhofer-Institut für Werkzeugmaschinen und Umformtechnik, IWU, Reichenhainer Straße 88, 09126 Chemnitz, Germany

Magnetic impulse welding (MPV) is one of the few methods that allows joining different kinds of metals with significantly differing melting temperatures. It is conducted by colliding two metal sheets at high velicities. A sound joint without embrittlement effects or the formation of critical amounts of intermetallic phases can be produced. The Al-Cu system is relevant for a variety of reasons. With the rise of electromobility, the need for cheap and light conductors like aluminum to be connected to copper is high. Furthermore, the results of the investigation of the joining mechanism between Al and Cu are relevant for systems like Al-Ti and Al-Fe, etc., whose welds are required for lightweight construction. The joining mechanisms of Al-Cu welds were mainly analyzed using scanning electron microscopy. The relevance of the occurring small amounts of intermetallic phases is determined by growing them via a heat treatment and comparing tensile testing results of heat treated and untreated welds. If a thin surface layer melts and resolidifies during the process, can be investigated with EBSD. With a variation of the process parameters the influence on the resulting microstructures and interfacial morphology has been studied.

MM 30.13 Tue 18:15 P4

Fracture Matching of Metals in Forensic Science — •Jens Balzer, Bert Weimar, Horst Katterwe, and Werner Deinet — Kriminaltechnisches Institut, Bundeskriminalamt, 65173 Wiesbaden

The comparison of marks caused by firearms and tools as well as of marks on fracture surfaces is of great importance in forensic sciences. Very often a forensic laboratory is asked to prove whether two or more pieces of a broken metal originally were part of one and the same object. Examiners magnify the marks using comparison light microscopes or comparison scanning electron microscopes. In a pattern fit analysis the matching is based on characteristic features of the fracture surface. Sometimes the question arises whether the degree of similarity is sufficient to make the statement that the two broken pieces were originally one.This corresponds in the toolmark case to the question, if two marks were produced by the same tool. For these, efforts have been made to obtain objective criteria for an identification using probability theory models. References: 1) Voss-de Haan, Katterwe, Simross *Physik in der Kriminaltechnik*, Physik Journal 2, 35, 2003; 2) Katterwe, Körschgen, Ahlhorn *Proceedings Marks*, ISBN 3-00-009338-9, Berlin 2001; 3) Katterwe *Fracture Matching*, AFTE Journal 37, 229, 2005; 4) Weimar, Katterwe, Braune *Formspuren* in Widmaier *Strafverteidigung*, Beck 2014; 5) Katterwe, Braune, Körschgen, Radke, Weimar *Comparison SEM in Forensic Science*, AFTE Journal 41, 283, 2009; 6) Stone *Probabilistic Model of Fractures in Brittle Metals*, AFTE Journal 36, 297, 2004; 7) Deinet, Katterwe *Probability Models*, AFTE Journal 39, 4, 2007.

MM 30.14 Tue 18:15 P4

Plane wave scattering on Janus spheres — •Jochen Wauer[1] and Tom Rother[2] — [1]Hochschule Neubrandenburg, University of Applied Sciences — [2]German Aerospace Center(DLR), Remote Sensing Technology Inst., Neustrelitz

Janus spheres are objects of growing interest in different fields of technology. They can be used in medicine for a precise drug positioning, and they hold an enormous potential for the development of new and active materials, just to mention only two applications of recent interest in nanotechnologies. Some of those Janus spheres are still industrially manufactured. It must be noted, however, that there exists a certain lack of knowledge about the scattering behavior of such objects although it might be of some interest not only for diagnostic purposes but also for discovering new applications. We present the application of the T-matrix method to solve the scattering problem of a plane electromagnetic wave on a dielectric sphere the surface of which is partially covered with a perfect metal. Additionally, the scalar scattering problem, i. e. the scattering of acoustic waves on different types of Janus spheres will be discussed. First results are presented, and an interesting effect for specially oriented Janus spheres at lower size parameters is discussed.

MM 30.15 Tue 18:15 P4

A school badge based on scalable structural color — •Shiyao Jia, Yudie Huang, Yi Wang, Wenxin Wang, Zhihang Wang, Jiaxu Chen, and Fanzhou Lv — Harbin Engineering Unversity,Harbin,China

The researches on alumina membrane already has hundreds of years, and owing to its highly ordered honeycomb structure, anti-corrosion, transparencyand mechanical properties, the alumina membrane has become a hot spot in nanotechnology in these years. Here, the optical interference at the interfaces of alumina membrane is used to selectively reflect the light and present the structural color, based on this theory, we made a vivid and colorful school badge. The thickness of alumina membranes are regulated by controlling the anodizing conditions precisely. Different light with specific frequency can be reflected by changing the thickness of alumina membranes, thus demonstrating the relevant structural color on corresponding areas and presenting the picture of school badge, which can be further developed as a nanophotonic device for sensing.

MM 30.16 Tue 18:15 P4

Oriented and isotropic electrospun magnetic nanofibers - experiment and simulation — •Timo Grothe[1], Jan Lukas Storck[1], Al Mamun[1], Marah Trabelsi[1,2], Michaela Klöcker[1], Christoph Döpke[1], Lilia Sabantina[1], Tomasz Blachowicz[3], and Andrea Ehrmann[1] — [1]Bielefeld University of Applied Sciences, Faculty of Engineering and Mathematics, 33619 Bielefeld, Germany — [2]Ecole Nationale d'Ingénieurs de Sfax, Sfax 3038, Tunisia — [3]Silesian University of Technology, Institute of Physics - Center for Science and Education, 44-100 Gliwice, Poland

Due to their strong shape anisotropy, magnetic nanofibers are of high interest in basic research as well as in spintronics, neuromorphic computing, for data storage, etc. Besides typical methods to prepare magnetic nanofibers, such as vapor growth, focused-ion-beam milling, or template-based methods, electrospinning allows for creating magnetic nanofiber mats [1].

Electrospun magnetic nanofibers, however, impose new challenges on micromagnetic simulations due to their varying diameters and bending radii. On the other hand, to allow for comparing simulated magnetization reversal processes with experimental findings, it is necessary to optimize the distribution of magnetic particles in the nanofibers.

Here we discuss different possibilities to tailor nanofiber diameters and shapes, influence the distribution of magnetic nanoparticles in the fibers as well as the nanofiber orientation inside the mat, and model static and dynamic properties of idealized and real nanofiber networks.

[1] C. Döpke et al., Nanomaterials 9, 92 (2019)

MM 30.17 Tue 18:15 P4

Comparison and analysis of ultra-narrow gaps fabricated by electron and helium ion beam lithography — Hao HU[1,2], Monika Fleischer[2], and •Pierre-Michel Adam[1] — [1]Universite de Technologie de Troyes, 12 Rue Marie Curie, CS42060, 10004 Troyes Cedex, France — [2]Institute for Applied Physics and Center LISA+, Eberhard Karls University Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Metal nanostructures with ultra-narrow gaps, which enable strong field enhancements in plasmonic structures, have attracted widespread attention in physics, chemistry, and biology. However, fabricating ultra-narrow nanogaps is still challenging at present, and controllable gap size, accurate dimensions, and scalable fabrication are desired for further applications. The most common methods for fabricating nanogaps arrays are electron beam lithography (EBL) and focused ion beam (FIB) milling. Depending on the difference of cross-linking reaction and degradation reaction occurring under the electron beam, the photoresist can be classified into two types: positive tone and negative tone. FIB can be divided into He-ion and Ga-ion beam depending on the ion source used. In this study, we provide a comparison of nanostructures fabricated with different methods including different types of EBL and FIB. By varying the fabrication methods of the nanostructures, we aim to find optimized approaches for fabricating ultra-narrow nanogaps.

MM 30.18 Tue 18:15 P4

Magnetoresistance of ruthenium nanogranular wires — •Nikolai Mai[1], Thomas Heinzel[1], Mihai Cerchez[1], Shibesh Dutta[2], Anshul Gupta[2], Shreya Kundu[2], Giacomo Talmelli[2], Florin Ciubotaru[2], Zsolt Tokei[2], and Christoph Adelmann[2] — [1]Heinrich Heine University Düsseldorf, Universitätsstr. 1, 40225, Düsseldorf — [2]Imec, 3001 Leuven, Belgium

Ruthenium is a promising candidate to replace Cu for metallic interconnects as electronics continues to scale down. Although the resistivity of Ru is less dependent on the thickness of the interconnect than that of Cu, the scaling problem in this case manifests with increased resistivity as the size of the interconnect becomes comparable to the size of the grain and to the mean free path. Here we present longitudinal and transversal magnetoresistance measurements and IV characteristics of Ruthenium nanogranular wires discussing the role of the grain-interface in the Ru-resistivity.

The wires with a cross section less than 150 nm^2 were obtained by a conformal atomic layer deposition of a 10 nm thick Ru film on SiO_2 cores (height 25 nm and width 300 nm) patterned on 300 mm Si (100) wafers, followed by an anisotropic reactive ion etch. The wires were protected by $SiN_x/SiO_2/SiN_x$ passivation layer, whereas the Al contacts were formed after passivation opening at the ends of the wires. The samples were at 420°C for 20 mins in forming gas.

MM 30.19 Tue 18:15 P4

Effect of Interfaces in the Oxide Transport Process in Platinum Coated Porous Frameworks of Yttria-Stabilized Zirconia (YSZ) — •Michele Bastianello[1], Jan-Ove Söngen[1], and Matthias T. Elm[1,2,3] — [1]Center for Materials Research, Justus-Liebig-University Gießen, Germany, Heinrich-Buff-Ring 16, 35392 Gießen — [2]Institute of Experimental Physics I, Justus-Liebig-University Gießen, Germany, Heinrich-Buff-Ring 16, 35392 Gießen — [3]Institute of Physical Chemistry, Justus-Liebig-University Gießen, Germany, Heinrich-Buff-Ring 17

Oxygen permeation membranes are of high interest for the production of pure oxygen. Such membranes need to transport not only oxygen ions but also the electronic charge carriers making mixed conducting oxide ceramics necessary. Research focusses mostly on multi-phase ox-

idic mixture or on high amounts of noble metals in oxide ceramics to achieve high mixed ionic and electronic conductivity. As an alternative approach, we hereby present the preparation of nano-structured composite materials using pulsed laser deposition (PLD) combined with atomic layer deposition (ALD). In particular, using PLD porous YSZ thin films were prepared and their surface was coated homogeneously with about 36 nm of Platinum using ALD. The transport properties of the composites were investigated using electrochemical impedance spectroscopy. To elucidate the influence of the interfaces, a series of multilayered YSZ-Pt-YSZ samples were prepared using PLD in order to obtain a fully controlled model system for comparison.

MM 30.20 Tue 18:15 P4

Optimization of structural and electrochemical properties of $LiNiO_2$ thin film cathodes — •Juri J.E. Becker, Fabian Michel, Hendrik Hemmelmann, Angelika Polity, and Matthias T. Elm — Center for Materials Research, Gießen, Germany

Due to its higher energy density layered lithium-nickel(III)-oxide (LNO) is a possible alternative to lithium cobalt oxide, which is used as cathode material in lithium-ion batteries (LIBs). However, LNO suffers from thermal instability as well as the fact that Ni^{2+}-ions have the tendency to substitute Li^{+}-ions during delithiation. To investigate the structural and electrochemical properties of LNO in more detail, thin films were prepared as model electrodes using radio frequency magnetron sputtering. For this purpose, a LNO target was pressed and thin films were deposited on a c-sapphire|platinum substrate. The influence of the growth temperature on the structural properties during the sputtering process was examined. At higher temperatures the crystallinity of LNO is increased which allows a better lithium-ion diffusion during the intercalation process. Pouch-cells were built using the deposited cathodes. Electrochemical measurements with a potentiostat reveal phase transitions occuring during the cycling process.

MM 30.21 Tue 18:15 P4

Ti3C2/MoS2 composite as anode material for lithium-ion batteries — •Peng Guo[1,2], Yuquan Wu[1], Lennart Singer[1], Peter Comba[2], and Rüdiger Klingeler[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Germany — [2]Inorganisch-Chemisches Institut, Universität Heidelberg, Germany

MXene, represented by Ti3C2, has received increasing attention when applied as anode material for lithium-ion battery due to its superior conductivity and hydrophilicity. Since the application of MXene is limited by its low capacity, in this work, a PDDA-assisted electrostatic attraction method was used to assemble a Ti3C2/MoS2 composite. The microscopic morphology, crystalline features and microstructure of the Ti3C2/MoS2 composite materials studied by X-ray diffraction (XRD) and field emission scanning electron microscopy (FESEM) are reported. Electrochemical studies reveal a specific capacity of 747 mAhg-1, at 400 mAg-1, of the Ti3C2/MoS2 composite electrode which notably increases to 776 mAhg-1 after 30 cycles.

MM 30.22 Tue 18:15 P4

Polypyrene tetraone (PPTO) as cathode material for lithium-ion batteries — •Jonas Spychala[1], Yuquan Wu[1], Lucas Ueberricke[3], Michael Mastalerz[3], and Rüdiger Klingeler[1,2] — [1]Kirchhoff Institute of Physics, Heidelberg University, Germany — [2]Centre for Advanced Materials, Heidelberg University, Germany — [3]Organisch-Chemisches Institut, Heidelberg University, Germany

Covalent organic frameworks (COFs) have emerged as promising candidates for cathode materials in lithium-ion batteries, due to their superior conductivity, electrochemical stability and structural richness. In order to assess the feasibility of Polypyrene tetraone (PPTO) for electrochemical energy storage, we have investigated its electrochemical properties by means of cyclic voltammetry (CV), galvanostatic cycling (GCPL), and electrochemical impedance spectroscopy (EIS). Cyclic voltammetograms show two characteristic redox pairs, at 2.4 V and 2.8 V, respectively, with small overpotentials. In comparison to the monomers which capacity amounts to 70 $mAhg^{-1}$ in the initial cycles, PPTO delivers significantly increased capacities of 140 $mAhg^{-1}$. This indicates that higher carbonyl utilization is achieved by polymerization. The capacity retention in PPTO by cycle 10 is 96% and 70% by cycle 50. The effects of different porosities and electrode fabrication procedures are discussed.

MM 30.23 Tue 18:15 P4

Phase transformation in Li4+xTi5O12 probed optically — •Yug Joshi, Robert Lawitzki, and Guido Schmitz — Chair of Materials Physics, Institute of Materials Science, University of Stuttgart, Stuttgart, Germany

The mechanism and the kinetics of the phase transformation from spinel structured Li4Ti5O12 to rock-salt type Li7Ti5O12 is studied by utilizing the electrochromic properties of the material. Thin films of Li4Ti5O12 are deposited on platinum-coated substrates using rf-ion beam sputtering. In-situ and ex-situ optical spectroscopy (in reflectance geometry) is performed along with electrochemical characterization. In-situ measurements demonstrate the reversible electrochromic behavior of the deposited thin films and the effect of the change of lithium content on the reflectance spectrum. The kinetics of the phase transformation is examined by probing the lateral diffusion lengths of lithium, optically revealed by the drastic blue color of the lithium-rich rock salt phase. Ex-situ measurements quantify the optical constants of the thin films for different charge states, by modeling the reflectance spectrum with a Clausius-Mossotti relation. The concentration dependence of the derived dielectric constants points out a fast lithium ion transport through the grain boundaries, thereby segregating a conductive lithium-rich phase at the grain boundaries. This is further confirmed by the change in the lateral diffusion lengths (reveled optically) with the varying grain sizes.

MM 30.24 Tue 18:15 P4

Template-Assisted Fabrication of Spectrum-Programmable Superlattice Photonic Crystals for Efficient Solar Energy Harvesting — •Zhiqiang Zeng, Rui Xu, Huaping Zhao, and Yong Lei — Technische Universität Ilmenau, 98693, Ilmenau, Germany.

Superlattice photonic crystals (SPhCs) possess tremendous potentials as building blocks for high-performance solar thermal conversion systems because of their great flexibility in optical manipulation. For practical utilization of SPhCs as solar absorbers, the key points are to fabricate large-scale highly-ordered SPhCs and to realize spectrally-programmable selective light absorption spectra. In this work, wafer-scale nickel (Ni) SPhCs are fabricated by structurally replicating alumina templates comprising two sets of nanopores (NPs) and nanoconcaves (NCs). Both self-aligned sets of NPs and NCs are simultaneously formed during the anodization of surface-patterned aluminum foils, consequently avoiding otherwise multi-step lithography and resulting in large-scale uniformity. The as-replicated Ni SPhCs demonstrate omnidirectional polarization-independent selective light absorption spectra whose cutoff wavelength can be precisely programmed in the spectral range of ~600 to ~1500 nm. Below the cutoff wavelength all absorption efficiencies are enhanced to over 90% due to surface plasmon resonance and cavity resonance stemming from both NCs and NPs. All these advantages in optics and fabrication qualify Ni SPhCs as excellent candidates of solar absorbers for practical utilization.

MM 30.25 Tue 18:15 P4

Non-adiabatic time-optimal edge mode transfer on mechanical topological chain — •Ioannis Brouzos[1], Georgios Theocharis[1], Ioannis Kiorpelidis[1], and Fotios Diakonos[2] — [1]Laboratoire Acoustique Universite Mans — [2]University of Athens

We show that it is possible to successfully transfer topologically protected edge modes across a mechanical chain, with non-adiabatic optimal control schemes, in a time even shorter than their own period. The proposed protocols vastly outperform the adiabatic ones, both in time-scales and in robustness against disorder. Our control schemes possess non-adiabatic time intervals during which driving frequencies exceed characteristic frequencies of the system, shift the value of adiabatic invariant, and exchange a great amount of energy. As a bonus feature and in contrast with quantum chains, ultrafast pumping in classical chains is accompanied with amplification of the edge mode. Introducing non-adiabatic pumping of topologically protected states aims to challenge common approaches in this emerging field.

MM 30.26 Tue 18:15 P4

Atomistic investigation of the LLZO / Li metal interface for all-solid state batteries — •Lisette Haarmann and Karsten Albe — Technische Universität Darmstadt, Otto-Berndt-Str. 3 64287 Darmstadt

In order to achieve maximal energy densities in all solid state Li ion batteries (ASSB), the introduction of a metallic Li anode is crucial. However, the interface kinetics between Li metal and the solid electrolyte is mostly unexplored and an atomistic picture is still missing. Therefore ab-initio calculations based on density functional the-

ory (DFT) are carried out in order to investigate the lithium transfer over this interface.

Aluminium doped $Li_7La_3Zr_2O_{12}$ (LLZO) is considered as a model system due to its stability against lithium metal and its minimal intrinsic interface resistance. Jump processes of lithium between the metal (atomic state) and the electrolyte (ionic state) and the accompanying charge transfers are investigated both with Nudged Elastic Band (NEB) calculations and ab-initio Molecular Dynamic (AIMD) simulations.

While the former provides activation energies for the jump processes, the latter allows the investigation of structural rearrangements at the interface above 0 K, as well as the calculation of lithium diffusion coefficients and preferred transport directions.

Combining the information of both approaches, the energy landscape of the LLZO / Li metal interface is constructed providing information on the lithium transport in an ASSB.

MM 30.27 Tue 18:15 P4

Hybrid Functionals in an all-electron FLAPW basis: challenges imposed by exa-scale supercomputers — •Matthias Redies[1,2], Gregor Michalicek[1], Christian Terboven[3], Daniel Wortmann[1], Matthias Müller[3], and Stefan Blügel[1] — [1]Forschungszentrum Jülich and JARA — [2]Department of Physics, RWTH Aachen University, 52056 Aachen, Germany — [3]IT Center, RWTH Aachen University, 52074 Aachen, Germany

Hybrid exchange-correlation functionals facilitate some of the most accurate DFT calculations and are especially important in systems, where traditional exchange-correlations functionals fail, such as oxides. However, this accuracy comes at a large computational cost. Until recently these calculations have been restrained to small system, due to the excessive demand for computing resources. This large computational demand makes hybrid functionals a suitable problem for the next generation of supercomputers.

On this poster we are going to present how we parallelize and adapt the FLEUR [1,2] code, an all-electron FLAPW implementation developed in Forschungszentrum Jülich, to perform hybrid functional calculations efficiently on next generation supercomputers and present a path towards utilizing heterogenous computing architectures.

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[1] www.flapw.de [2] Friedrich *et al.*, J Phys: Condens Matter. **24(29)**:293201. [3] www.max-centre.eu

MM 30.28 Tue 18:15 P4

Nonequilibrium dynamics of laser excited SiC: Description of Laser excited SiC with the help of an electronic temperature dependent interatomic potential — •Malwin Xibraku, Bernd Bauerhenne, and Martin Garcia — Heinrich-Plett-Straße 40, 34132 Kassel

Silicon carbide (SiC) nanocrystals are of great interest in medicine, because of their pleasant properties, such as biocompability, high chemical and thermal stability. These nanocrystals can be very well generated using ultrashort laser pulses. Density Functional theory (DFT) has proven to be a appropriate tool to describe the influence of ultrashort laser pulses on solids due to the accurate quantum mechanical treatment of electrons. Due to the fact that 48 million particles are already contained in a cube SiC of side length 100 nm, such a system cannot be computed with DFT. Therefore, the aim of this work is to describe the forces between the atoms in the SiC cube by an effective electronic temperature (Te) dependent interatomic potential. Te is taken into account for including the effect of the laser-excited electrons. Recently, we found such a potential for silicon (Si) and carbon (C). In this work, a potential for siliconcarbite (SiC) was constructed. This potential reduces to the existing potentials for silicon (Si) or carbon (C), if only silicon (Si) or carbon (C) particles are present, respectively.

MM 30.29 Tue 18:15 P4

Molecular dynamics study of impact welding processes — •Benedikt Philipp Eggle-Sievers, Tobias Stegmüller und Ferdinand Haider — Universität Augsburg, Institut für Physik, Universitätsstraße 1 86159 Augsburg

Impact welding processes like explosive welding or magnetic pulse welding allow for the joining of different materials in a fast and reliable fashion. In the presented work, such joints between Al and Cu are investigated by the means of molecular dynamics simulations. The process of impact welding is divided into two stages, the loading and the unloading stage. The MD model consists of two plates forming a typical impact angle between 5° and 30°. Besides the impact velocity, typically being several hundreds of meters per second, the angle is the parameter to vary. Another investigated phenomenon is the formation of a jet between both plates. It is an open question of ongoing research, whether the jetting can be traced back to the surrounding atmosphere, or to flaking and local melting of the material whilst the collision. In the presented work, the influence of the brittle oxide layer on the Al-surface is considered, requiring advanced potentials with the capability to capture the properties of metallic as well as of covalent–ionic bonds.

MM 30.30 Tue 18:15 P4

Ab Initio **Molecular Dynamics Simulations of Chemical Processes at the Crack Tip** — •Tobias Müller and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Fracture of materials takes place in an environment, usually air or liquid water. When a crack propagates, the newly created surfaces become exposed to the molecules of the surrounding gas phase or liquid, e.g. oxygen and water, which leads to a series of chemical processes. For example, the molecules can attack a stretched bond at the crack tip, giving rise to chemically activated bond breaking and resulting in subcritical crack growth and stress corrosion cracking. In order to encompass the complex chemical interplay between bond breaking at the crack tip and the adsorption/bond saturation with molecules from the environment, unbiased and accurate quantum-chemical methods are needed. Here we show first *ab initio* molecular dynamics simulations for silicon to study stress corrosion cracking by subcritical loads. A series of Car-Parrinello molecular dynamics (CPMD) simulations were performed with different loads and for crack tips exposed to hydrogen, oxygen or water.

MM 30.31 Tue 18:15 P4

Development of an analytic bond-order potential for Fe-Co — •Aleksei Egorov, Aparna Subramanyam, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

The growing demand for soft magnets and the potential for magnetic topological structures continue to draw attention to Iron-Cobalt (Fe-Co) alloys. The description of the magnetic degrees of freedom for the calculation of the phase diagram and microstructural properties are still a challenge for atomistic simulations. Quantum-mechanical approaches capture the details of the magnetic interactions, but are typically too computationally expensive for large scale simulations or extensive sampling of spin space at finite temperature. The computationally less demanding classical approaches usually cannot provide a reliable description of the influence of magnetism. Here we report the development of an analytic bond-order potential (BOP) for Fe-Co that provides a robust description of magnetism in large-scale simulations.We parameterize the analytic BOP with reference data obtained by density functional theory (DFT) calculations using two parameterization strategies: i) chemical morphing of an existing BOP for Co towards Fe by varying the band filling and ii) successive parameterization of the BOP parameters starting from DFT-based Hamitlonian matrix elements. We use the obtained BOP models to study the band filling trends of structural stability and the volume dependence of the magnetic moment. The results are compared to the available experimental and DFT data and analyzed with canonical band theory.

MM 30.32 Tue 18:15 P4

The Process for Creating A General-Purpose Machine Learned Potential for Silicon Carbide — •Harry Tunstall, James Kermode, and Gabrele Sosso — The University of Warwick, Coventry CV4 7AL, United Kingdom

SiC is a prototypical material for high temperature applications (e.g aerospace, automotive and thermoelectric) involving complex microscopic processes typically inaccessible to experiments. To gain insight into the functional properties of e.g. SiC nanostructures, computationally expensive quantum mechanical methods such as density functional theory (DFT) must be employed. This is because less computationally demanding methods are almost always not accurate enough. In fact, similar to Si and C alone, various empirical interatomic potentials have been developed for SiC, such as Tersoff or Stillinger-Weber. These potentials are designed to reproduce specific features of the material, at the expense of transferability to a wider range of functional properties.

The aim of this project is to build a general purpose interatomic potential for SiC (e.g using machine-learning regression, in the form of Gaussian approximation potentials (GAPs) and neural networks

(NNs), starting from a DFT dataset of representative configurations), enabling accurate large scale simulations into defects and grain boundaries. The methodology for creating and maintaining a machine learning database for atomic systems from the ground up will be discussed, from the perspective of this ongoing project.

MM 30.33 Tue 18:15 P4

Density functional study of metal and metal-oxide (Cu, Ni, Co, Fe, Mn) nucleation and growth on the anatase TiO_2(101) surface — •Leila Kalantari, Fabien Tran, and Peter Blaha — Institute 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 oxide (MO_x) nanoparticles attached on anatase TiO_2 surface. In this work, we performed density functional theory calculations to provide a detailed description of geometry, electronic properties and catalytic sites. The adsorption of M_xO_y(M=Cu, Ni, Co, Fe and Mn) and (x = 5, y = 0-5) clusters on the TiO_2(101) surface has been studied using the PBEsol exchange correlation functional with a Hubbard correction (U). Various geometries of metals and metal-oxide have been investigated. It is found that, unsaturated 2-fold-coordinated oxygen sites may serve as nucleation centers for the growth of metal cluster and the adsorption of Ni atoms on the anatase surface is stronger than of other atoms. Energetically, the NiO cluster prefers the bridge site formed by 2-fold-coordinated oxygen atoms with an adsorption energy of 3.55 eV. We found that the Ni_nO_n adsorption energy remains about constant with cluster size n which makes the formation of bigger clusters plausible as confirmed by TEM images. Ni has a more stable configuration with less oxygen, while for other metals the adsorption energy remains almost constant or is reduced with less oxygen specially in Mn, which is in agreement with the experimental results.

MM 30.34 Tue 18:15 P4

Neural network for learning and predicting tight-binding parameters — •Till Hanke, Jürgen Henk, and Ingrid Mertig — Martin-Luther-Universität Halle-Wittenberg

Tight-binding approaches have two major advantages: they allow for an intuitive interpretation of electronic structures and to perform large-scale electronic-structure calculations. However, parameter sets, either DFT-based or empirical, are often available only for simple bulk systems.

We report on artificial neural networks which can predict Slater-Koster tight-binding parameters for heterogeneous systems. The networks are trained using parameter sets for elemental materials. These sets will be used for electronic-structure and transport calculations (on the femtosecond timescale) for which accurate descriptions of complex interfaces are essential.

MM 30.35 Tue 18:15 P4

High-dimensional neural network potential for laser-excited materials — •Pascal Plettenberg, Bernd Bauerhenne, and Martin E. Garcia — Theoretical Physics, University of Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

In recent years, machine learning techniques have been increasingly used to develop highly accurate representations of ground state or single excited state potential energy surfaces (PES) for large systems. Here, we want to develop such a machine learning potential to electronic temperature (T_e) dependent PES of solids excited by intense femtosecond laser pulses. Studying the effects of ultrashort excitation on the long-term (nanoseconds) and large-scale (hundreds of nanometers) dynamics of a material has not been possible so far, because ab-initio simulations are limited to a small number of atoms and short time scales. On the other side, T_e-dependent interatomic potentials, which can be efficiently used in large-scale simulations, are difficult to derive and often do not reach the required accuracy. In this work we investigate the possibility to fill this gap of simultaneous efficiency and ab-initio accuracy with a high-dimensional neural network potential including an electronic temperature dependency, which is implemented as an additional input node. We train the network to reference Density-Functional-Theory data of thin-film silicon and demonstrate its performance in molecular dynamics simulations.

MM 30.36 Tue 18:15 P4

Application of Machine Learning Interatomic Potentials to Carbon Nanostructures — •Tom Rothe[1], Erik Lorenz[1,2], Gustav Johansson[3], Fabian Teichert[1], Daniel Hedman[3], Andreas Larsson[3], and Jörg Schuster[1,2] — [1]Chemnitz University of Technology, Chemnitz, Germany — [2]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany — [3]Luleå University of Technology, Luleå, Sweden

Machine Learning Interatomic Potentials (ML-IAPs) are a new class of non-empirical IAPs for atomistic simulations that are created using Machine Learning methods. Promising near quantum mechanical accuracy while being orders of magnitudes faster than first principle methods, they are the new "hot topic" in material simulation research.

This work investigates the state of the research in the field of ML-IAPs for simulation of carbon nanostructures (CNS). Publicly available ML-IAPs are used for simulation of defect induced deformation of carbon nanotubes. Comparing the results with previously published density-functional tight-binding results and our own empirical IAP geometry optimizations show that ML-IAPs can already be used for simulations of CNS. They are indeed faster than and nearly as accurate as first-principle methods.

We also present results for a new Neural Network-based ML-IAP trained on graphene, haeckelite, carbon nanotube, and fullerene structures, with and without defects.

MM 30.37 Tue 18:15 P4

a Neural Network Potential with electrostatic interaction — •Tsz Wai Ko and Jörg Behler — Universität Göttingen, Institut für Physikalische Chemie, Theoretische Chemie, Tammannstraße 6, 37077 Göttingen, German

High-dimensional neural network potentials (HDNNPs), which represent one of the most frequently used types of ML potentials, construct the short-range energy as a sum of environment-dependent atomic energy contributions. In addition, long-range electrostatic interactions can be included employing environment-dependent atomic charges. Both contributions are determined using atom-centered radial and angular symmetry functions as local structural descriptors.

Here we present benchmark calculations for several model systems such as water molecules and Zinc oxide clusters using Density Functional Theory reference calculation

MM 30.38 Tue 18:15 P4

Machine-learning Driven Global Optimization of Atomic Surface Structures — •Sami Kaappa and Karsten Wedel Jacobsen — CAMD, Department of Physics, Technical University of Denmark, 2800 Kongens Lyngby, Denmark

Efficient global optimization of atomic structures is a long-pursued objective in material sciences since the required number of *ab initio* calculations is usually computationally infeasible. In this work, a machine-learning guided approach is utilized to model the potential energy hypersurface (PES) as a function of atomic coordinates, and the surrogate model is used to intelligently sample the search space for the global minimum in order to reduce the number of expensive DFT calculations. In the method, the translational and rotational symmetries as well as symmetries with respect to interchanging positions of alike atoms are naturally inherited by a global fingerprint, and both energy and force information of DFT calculations are used in the Gaussian process machinery to model the PES. We will present both the performance of the method in comparison to previously reported, similar procedures, and predicted global minima for certain atomic structures where the optimal atomic configuration is not trivial. Although DFT calculations are carried out here, we note that higher-level theories can be used as well to probe energies and forces of single structures, to be offered as training data for the model.

MM 30.39 Tue 18:15 P4

Symmetry-adapted Hamiltonian representations for machine-learning-based tight-binding parametrization — •Michael Luya[1] and Reinhard Maurer[2] — [1]Department of Mathematics, University of Warwick, Coventry, UK — [2]Department of Chemistry, University of Warwick, Coventry, UK

To tackle modern materials challenges, high efficient and accurate electronic structure methods need to be available that reliably predict the atomic structure, electronic and spectroscopic properties of materials at ever larger scales. Machine-learning methods have recently revolutionised the construction of interatomic potentials in computational materials science and are increasingly considered for the efficient construction of effective electronic structure methods such as tight-binding. Here we explore two-centre, three-centre and crystal field parametrisations of Hamiltonians in local basis representations

that conserve important symmetries including rotational equivariance properties and permutational invariance. We show that this representation can accurately map on-site and off-site Hamiltonian contributions extracted from Density Functional Theory. We also investigate the physical significance of these parameters and the prospect of integration into deep-learning based parametrisation schemes.

MM 30.40 Tue 18:15 P4

X-ray reflectivity of thin films evaluated by neural networks — Thorben Finke and •Uwe Klemradt — II. Physik. Inst., RWTH Aachen University, Germany

X-ray reflectivity (XRR) is a widespread method for the structural analysis of thin films on the nanometer scale. We studied the application of a neural network based on Tensorflow for the evaluation of reflectivity curves from metal films of several 10 nm thickness on Si substrates. The focus was on the automatic fitting of layer thickness and surface / internal interface roughness. The network was trained using 900k simulated XRR curves and provided highly accurate results in subsecond computation time, resulting in thickness and roughness errors below 0.1 nm in 95% of the cases when applied to data not known to the network. The results will be discussed in the context of automatic fitting with minimum user interference and high-throughput experiments.