MM 12: Poster I

Time: Monday 18:15–20:00 Location: P2/OG1+2

MM 12.1 Mon 18:15 P2/OG1+2

Time-of-Flight X-ray Photoelectron Microscopy (ToF-X-PEEM) — •G. Schönhense[1], O. Tkach[1,2], O. Fedchenko[1], Y. Lytvynenko[1], D. Vasilyev[1], Q.L. Nguyen[3], T.R.F. Peixoto[4], A. Gloskovskii[4], S. Chernov[4], M. Hoesch[4], N. Wind[4,5], M. Heber[4], C. Schlueter[4], C. Sharma[5], K. Rossnagel[4,5], M. Scholz[4], and H.-J. Elmers[1] — [1]Mainz Univ. — [2]Sumy State Univ. — [3]SLAC Nat. Accel. Lab., USA — [4]DESY Hamburg — [5]Kiel Univ.

The classical solution for photoelectron imaging in the X-ray range (X-PEEM) employs a hemispherical analyzer, as first described by Tonner1. X-PEEM shows reduced spatial and energy resolution and notoriously low transmission, a consequence of the slits and small angular acceptance of the hemisphere. ToF-X-PEEM combines time-of-flight energy recording with a new lens optics minimizing spherical aberration. Systematic ray tracings predict a resolution in the (sub-) micron range, when a k-confining aperture array is placed in the second reciprocal plane, where the k-magnification can be zoomed in a large range. The new optics has been recently commissioned at PETRA-III (soft X-rays), studying ultrathin flakes and Moiré sandwich patterns of various transition-metal dichalcogenides. We demonstrate the high quality of deposited flakes by systematic ToF-X-PEEM characterization. Imaging large field of view >3mm with widened X-ray beam profile enables rapid chemical mapping with frame rates up to 1/s for strong core levels. Contracting the beam spot to <20mu and placing it on the desired flake allows small-area SX-ARPES employing the momentum-microscopy mode. [1] B.Tonner, NIMS A291, 60(1990)

MM 12.2 Mon 18:15 P2/OG1+2

Chlorine Corrosion of Superheater Steels — •Matthias Kroh, Sebastian Pentz, Ferdinand Haider, and Georg Krupkov — Univ. Augsburg, Inst. f. Physik, 86159 Augsburg

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

MM 12.3 Mon 18:15 P2/OG1+2

Nanoscale heat transport in heterostructures measured with UXRD at European XFEL — •Jan-Etienne Pudell[1,2,3], Marc Herzog[2], Max Mattern[2], Jasmin Jarecki[2], Alexander von Reppert[2], Ulrike Boesenberg[1], Angel Rodriguez-Fernandez[1], Wonhiuk Jo[1], Roman Shayduk[1], Wei Lu[1], Gregory Malinowski[4], Michel Hehn[4], Matias Bargheer[2,3], and Anders Madsen[1] — [1]European XFEL, Germany — [2]Institut für Physik und Astronomie, Universität Potsdam, Germany — [3]Helmholtz-Zentrum Berlin, Germany — [4]Institut Jean Lamour, Université Lorraine, France

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

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

MM 12.4 Mon 18:15 P2/OG1+2

Structural evolution and atomic transport in severely deformed bi-metallic samples — •Shraddha V. Sevlikar, Gerhard Wilde, and Sergiy V. Divinskiy — Westfälische Wilhelms-Universität Münster, Institut für Materialphysik, Münster, Germany

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

MM 12.5 Mon 18:15 P2/OG1+2

Study of Electron Transport in a DNA model — •Jorge Cardenas-Gamboa[1], José García[2], and Solmar Varela[1,3] — [1]Yachay Tech University, School of Chemical Sciences & Engineering, 100119-Urcuquí, Ecuador — [2]Institu Català de Nanociència I Nanotecnología(ICN2) ,08193-Barcelona, España — [3]Institute for Materials Science and Nanotechnology, Technische Universität Dresden. Dresden 01062, Germany

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

MM 12.6 Mon 18:15 P2/OG1+2

Investigations on thermal contact conductance between filled polymer composites and solids using micro thermography — •Oliver Roser[1,2], Andreas Griesinger[3], and Othmar Marti[2] — [1]Center for Heat Management (ZFW), Stuttgart — [2]Institute of Experimental Physics, Ulm University — [3]Baden-Wuerttemberg Cooperative State University (DHBW) Stuttgart

When optimizing cooling paths in electronic devices, thermal interface materials (TIMs) are used to optimize the thermal transfer between two solid surfaces. TIMs are thermally conductive filled polymer composites with a complex microstructure. We investigated the intrinsic thermal conductivity of TIMs and the thermal contact conductance between TIMs and solid substrate surfaces using micro thermography. The physical principles of thermal transport when considering this kind of contact have not yet been investigated in detail and just a few experimental results are available. Most common measurement techniques determine a macroscopic conductance. Random surface and filler structures however, cause several variations and some specific effects on contact conductance, which need to be investigated on a microscale. With the utilized IR camera system, we can take pictures

with a resolution of down to 14 microns per pixel. The new method allows us to analyze the microscopic heat paths on the particle scale and to understand the physical principles of heat transport in contact zones of TIMs. The main parameters which affect the contact conductance were identified and will be presented in addition to comparisons to other measurement methods, and a microscale simulation approach.

MM 12.7 Mon 18:15 P2/OG1+2

Hydrogen Diffusion in High-Pressure Torsion (HPT) deformed Magnesium and Magnesium-alloys — •Giorgia Guardi[1], Sabine Schlabach[1,2,3], Julia Ivanisenko[2,3], Stefan Wagner[1], and Astrid Pundt[1] — [1]Karlsruhe Institute of Technology, Institute for Applied Materials, Karlsruhe, Germany — [2]Karlsruhe Institute of Technology, Institute of Nanotechnology, Karlsruhe, Germany — [3]Karlsruhe Institute of Technology, Karlsruhe Nano Micro Facility, Karlsruhe, Germany

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

MM 12.8 Mon 18:15 P2/OG1+2

A systematic investigation of metastable phases in Niobium using density-functional theory — •Susanne Kunzmann[1], Gabi Schierning[1], and Anna Grünebohm[2] — [1]Universität Bielefeld, Germany — [2]Ruhr-Universität Bochum

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

The present work attempts to approach these previously unexplained observations in a multifaceted manner. Using density functional theory we investigate low energy metastable phases, their instability against deformation and potential transition paths to bcc ground state for selected phases and the influence of Tantalum contamination. We find both A15 and Pnma phases to be potential candidates for distorted Niobium, as they are low in energy and we discuss a simple transition path with a low energy barrier for the latter.

MM 12.9 Mon 18:15 P2/OG1+2

Computational local point-based boundary conditions method for eigenfrequencies in microwave eccentric spherical cavities — •Zoya Eremenko[1], Igor Volovichev[1], Oleksiy Breslavets[1], and Grigorios Zouros[2] — [1]O. Ya. Usikov Inst. for Rad. & Electr. Nat. Acad. of Sci. of Ukraine Kharkiv, Ukraine — [2]School of Electrical & Comp. Eng. Nat. Tech. Univ. of Athens, Athens, Greece

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

MM 12.10 Mon 18:15 P2/OG1+2

Machine learning force fields in VASP — •Ferenc Karsai[1], Andreas Singraber[1], Jonathan Lahnsteiner[1], Ryosuke Jinnouchi[2], and Georg Kresse[2] — [1]VASP Software GmbH, Sensengasse 8, Vienna, Austria — [2]University of Vienna, Department of Physics, Kolingasse 14-16, Vienna, Austria

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

MM 12.11 Mon 18:15 P2/OG1+2

Structure prediction of iron hydrides at high pressures by machine-learned interatomic potentials — •Hossein Tahmasbi[1], Kushal Ramakrishna[1], Mani Lokamani[1], Mandy Bethkenhagen[2], and Attila Cangi[1] — [1]Center for Advanced Systems Understanding (CASUS), HZDR, Görlitz, Germany — [2]CNRS, ENS de Lyon, Laboratoire de Géologie, Lyon, France

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

MM 12.12 Mon 18:15 P2/OG1+2

Machine Learning Interatomic Potentials for amorphous mesoporous metallosilicates — •Julian Greif, Konstantin Gubaev, and Blazej Grabowski — Universität Stuttgart, D-70049, Stuttgart, Germany

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

MM 12.13 Mon 18:15 P2/OG1+2

Deep learning for generation of optimal reaction environments — •Rhyan Barrett[1] and Julia Westermayr[2] — [1]Leipzig University — [2]Leipzig University

The design of reaction environments to reduce activation energies holds enormous potential for advancing many areas of chemical engineering but remains a difficult task due to the high combinatorial complexity of different conditions that influence a reaction. Herein, we use a cutting-edge deep learning model to enable the optimization of reactions. Initially we use a model to generate an abstract electrostatic field that reduces the activation barrier of a given reaction. We then look to optimize the ratio of continuum solvents to match the influ-

ence of the optimal electrostatic field generated by the model. The advantage of our method is that it is not limited to the initial solvent selection since any designed mixture will be compared with the global optimum electrostatic field produced by our model. The potential of the method will be demonstrated by optimization of the Claisen rearrangement reaction of allyl-p-tolyl ether and construction of an optimal environment but is generally applicable to any organic reaction.

MM 12.14 Mon 18:15 P2/OG1+2

Efficient graph neural networks for accurate interatomic potentials between surfaces and adsorbed atoms — •Nian Wu[1], Fabio Priante[1], Eric Kramer Rosado[1], and Adam S Foster[1,2] — [1]Department of Applied Physics, Aalto University, 00076, Espoo, Finland — [2]WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan

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

MM 12.15 Mon 18:15 P2/OG1+2

Investigation of bonding mechanism between early transition metals and antimony — •Carolin Petersen, Christian Stenz, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University

Using density functional theory (DFT) one can calculate the number of electron transferred (ET) and electron shared (ES) for crystalline materials. By plotting ET and ES for different materials on the x- and y- axes, the so-called bonding map is created. It can categorize the different bonding mechanisms, like covalent, ionic, metallic or metavalent and can predict properties such as the band gap, effective coordination number, electrical conductivity, or Born effective charge.

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

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

MM 12.16 Mon 18:15 P2/OG1+2

DFT structural characterization of β- and δ- intermetallic Al-Fe-Si phases — •Nebahat Bulut[1], Hanka Becker[2], Andreas Leineweber[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, Germany — [2]TU Bergakademie Freiberg, Institute of Materials Science, Germany

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

[1] P. Giannozzi et al., J.Phys.Condens.Matter 21, 395502 (2009)
[2] Becker et al. J. Alloys and Comp. 911 (2022) 165015

MM 12.17 Mon 18:15 P2/OG1+2

A method for charge-sloshing free precise linear-scaling density-functional calculations — •Rudolf Zeller — Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

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

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

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

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

MM 12.18 Mon 18:15 P2/OG1+2

How to Train a Neural Network Potential — •Alea Miako Tokita[1,2] and Jörg Behler[1,2] — [1]Lehrstuhl für Theoretische Chemie II, Ruhr-Universität Bochum, 44780 Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, 44780 Bochum, Germany

High-Dimensional Neural Network Potentials (HDNNPs) provide potential energy surfaces (PESs) with the accuracy of electronic structure calculations at strongly reduced computational costs, which enables extended molecular dynamics simulations of large systems. They are trained on reference energy and force data to learn an approximate but accurate functional relation between the atomic structure and the PES. However, due to the non-physical functional form, which is shared with many other types of machine learning potentials, this training and the validation of the potential have to be done with great care. In this contribution the construction of HDNNPs will be explained step by step including a discussion of possible pitfalls and tricks of the trade.

MM 12.19 Mon 18:15 P2/OG1+2

PyRamanGUI: An open-source multi-purpose tool to analyze Raman spectra — •Simon Brehm, Cameliu Himcinschi, Jakob Kraus, and Jens Kortus — TU Bergakademie Freiberg, Germany

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

MM 12.20 Mon 18:15 P2/OG1+2

Non-contact friction on various material systems — •Kim Lambert[1], Niklas Weber[1], Matthias Krüger[2], and Cynthia Vokert[1] — [1]Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen

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

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

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

MM 12.21 Mon 18:15 P2/OG1+2

Thermodynamical Stability Analysis of a Model Quasicrystal — •Moritz Holzwarth, Johannes Roth, and Hans-Rainer Trebin — FMQ, Uni Stuttgart, Germany

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

MM 12.22 Mon 18:15 P2/OG1+2

Excitation-induced non-thermal effects in silicon — •Simon Kümmel, Dominic Klein, and Johannes Roth — FMQ University of Stuttgart, Germany

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

MM 12.23 Mon 18:15 P2/OG1+2

Towards understanding the chemical bonding of unconventional metals — •Christian Stenz, Johannes Holters, and Matthias Wuttig — Institute of Physics IA, RWTH Aachen University, 52074 Aachen, Germany.

Solids can be distinguished based on their properties such as the band gap, effective coordination number, electrical conductivity, Born effective charge and so on. Based on these properties a classification into metallic, covalent, ionic and metavalent bonding seems appropriate. Metavalent bonding is a distinct bonding mechanism characterized by a competition between electron localization and electron delocalization. Chalcogenides like GeTe and Sb_2Te_3 and pnictides like Sb employ this bonding mechanism and can be characterized as 'incipient metals'. This raises the question if there are related metals, which are characterized by the same competition between electron localization and electron delocalization. We thus have been looking for such unconventional metals and focus on compounds of Te with transition metals. The overlap between Te p- and transition metal d- orbitals gives rise to a configuration which resembles the p-p σ-bond in incipient metals. Hence we are looking for related fingerprints such as soft, anharmonic bonds, an unconventional bond rupture and other characteristics which are found for incipient metals.

MM 12.24 Mon 18:15 P2/OG1+2

An efficiently automated method to sample the energies of grain boundaries — •Timo Schmalofski[1], Martin Kroll[2,3], Rebecca Janisch[1], and Holger Dette[3] — [1]ICAMS, Ruhr-University Bochum — [2]Department of Mathematics, Physics, and Computer Science, University of Bayreuth — [3]Department of Mathematics, Ruhr-University Bochum

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

MM 12.25 Mon 18:15 P2/OG1+2

Cubic scaling GW in the exciting code — •Manoar Hossain[1], Alexander Buccheri[1], Andris Gulans[2], and Claudia Draxl[1] — [1]Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin Germany — [2]Department of Physics, University of Latvia, Riga, Latvia

The GW approximation is the state-of-the-art method to incorporate many-body effects through the self-energy correction to the Kohn-Sham single-particle states. A serious drawback is that it becomes often computationally prohibitive due to its typical quartic dependence on system size. This restricts its use to systems with a few tens of atoms, highlighting the need to develop computationally efficient algorithms to extend the computation of the quasi-particle electronic structure to materials consisting of hundreds of atoms. In this work, we present a cubic-scaling algorithm implementation of the GW approximation in the exciting[1] code which is based on the linearized augmented planewave method. Our implementation employs the real-space imaginary-time formalism[2, 3] and relies heavily on Fast Fourier Transforms and efficient linear-algebra operations. To this extent we develop and make use of high-performance libraries, within the NOMAD CoE[4] with the aim to bring GW to exascale performance.

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

MM 12.26 Mon 18:15 P2/OG1+2

Physics Informed Neural Networks based Solvers for the Time-Dependent Schrödinger Equation — •Karan Shah and Attila Cangi — Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf, Görlitz, Germany

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

MM 12.27 Mon 18:15 P2/OG1+2

High-throughput calculations for property maps of solids — •Daniela Ivanova[1], Daniel Wortmann[1], Stefan Blügel[1], Matthias Wuttig[2], and Carl-Friedrich Schön[2] — [1]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany — [2]Department of Physics, RWTH Aachen University, Aachen, Germany

Over the last two decades, high-throughput computations have become a vital pillar of the scientific research and development process in the field of computational science. In order to forecast material properties for larger sets of atomic configurations, Density Functional Theory (DFT) has been employed as an automated, robust,

and highly-predictive first-principles approach. In this work, the DFT code Quantum ESPRESSO is deployed through the open source Automated Inter-active Infrastructure and Database for Computational Science AiiDA framework. Aside from the existence of (1) covalent, (2) metallic, and (3) ionic bonding, as well as the two weaker forms of (4) hydrogen and (5) van der Waals bonding, compelling evidence has recently been found for another bonding mechanism in solids such as crystalline chalcogenides, termed as (6) 'metavalent bonding'. Effective mass calculations promise essential data for mapping distinctions between the bonding mechanisms along the materials data set chosen for high-throughput computing.

MM 12.28 Mon 18:15 P2/OG1+2

A high-level workflow-based approach towards the exploration of magnetocaloric Heusler alloys by automated high-throughput simulations — •Simon Bekemeier[1], Alisa Chirkova[1], and Christian Schröder[1,2] — [1]Bielefeld Institute for Applied Materials Research, FH Bielefeld — [2]Faculty of Physics, Bielefeld University

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

MM 12.29 Mon 18:15 P2/OG1+2

Ontology-Template-Based Description of Anisotropic Conductivity Measurements — •Lennart Schwan[1,2], Michael Feige[2], Moritz Bluhm[3], Basil Ell[3], Andreas Hütten[2], and Sonja Schöning[1] — [1]Bielefeld Institute for Applied Materials Research (BIfAM), Bielefeld University of Applied Sciences, Department of Engineering Sciences — [2]Thin Films & Physics of Nanostructures, Bielefeld University, Department of Physics — [3]Semantic Computing Group, Bielefeld University, Faculty of Technology

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

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

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

MM 12.30 Mon 18:15 P2/OG1+2

An Ontology of Magnetocaloric Materials Research — Simon Bekemeier[1], Moritz Blum[2], Luana Caron[3], Philipp Cimiano[2], Basil Ell[2], Inga Ennen[3], Michael Feige[1], Thomas Hilbig[1], Andreas Hütten[3], Günter Reiss[3], Tapas Samanta[3], Sonja Schöning[1], Christian Schröder[1,3], Lennart Schwan[1,3], and •Martin Wortmann[3] — [1]Bielefeld Institute for Applied Materials Research, University of Applied Sciences Bielefeld, Interaktion 1, 33619 Bielefeld, Germany — [2]Faculty of Technology and CITEC, Inspiration 1, 33619 Bielefeld, Germany — [3]Faculty of Physics, Bielefeld University, 33501 Bielefeld, Germany

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

MM 12.31 Mon 18:15 P2/OG1+2

Laser processing of metal materials created by additive technologies. Optimization of structure and mechanical properties — •Iryna Galstian[1], Evgen Len[1], Tobias Gustmann[2], and Nicole Geissler[2] — [1]G. V. Kurdyumov Institute for Metal Physics of the N.A.S.U. Kyiv, Ukraine — [2]IFW Institute for Complex Materials. Dresden, Germany

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

MM 12.32 Mon 18:15 P2/OG1+2

MD Simulation of 3D Laser Printing — •Jonas Schmid, Kevin Vietz, Dominic Klein, and Johannes Roth — FMQ University of Stuttgart, Stuttgart, Germany

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

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

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

MM 12.33 Mon 18:15 P2/OG1+2

Molecular dynamics simulation of additive manufacturing: A highly non-equilibrated business — •Kevin Vietz, Azad Gorgis, Dominic Klein, and Johannes Roth — FMQ University of Stuttgart, Germany

Powder-bed additive manufacturing is a process that melts the powder with a laser beam, layer upon layer. By performing this melting-solidification process several times, one can build three-dimensional samples. This process is known as 3D printing. Up to now, most simulation studies on additive manufacturing rely on pure metals in vacuum. To fill this gap, we investigate the influence of argon gas on pure metals and explore the suitability of binary alloys for vari-

ous initial cluster structures, such as core-shell-clusters. We perform large-scale molecular dynamics simulations to depict the highly non-equilibrium material dynamics and evaluate our results by analyzing defects and properties on microscopic and macroscopic scales. Results show that the argon gas stabilizes the system and new material compositions could enhance the variety of applicable materials for additive manufacturing.

MM 12.34 Mon 18:15 P2/OG1+2

Atomistic simulations of crack-tip interface interactions in lamellar TiAl microstructures — •Onur Can Sen and Rebecca Janisch — ICAMS, Ruhr-University Bochum, Germany

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

MM 12.35 Mon 18:15 P2/OG1+2

Overview of Crack-Heterogeneity Interactions at the Atomic Scale — •Leon Pyka[1], Tarakeshwar Lakshmipathy[2], and Erik Bitzek[2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Department Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

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

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

MM 12.36 Mon 18:15 P2/OG1+2

Fracture surface energy of glasses obtained from crystalline structure and bond energy data — •Marco Holzer[1], Tina Waurischk[1], Janine George[1,2], Robert Maass[1,3], and Ralf Müller[1] — [1]Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany — [2]Institute of Condensed Matter Theory and Solid-State Optics at Friedrich Schiller University, Jena, Germany — [3]Department of Materials Science and Engineering at University of Illinois, Urbana-Champaign, USA

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

MM 12.37 Mon 18:15 P2/OG1+2

An in situ crack detection approach in additive manufacturing based on acoustic emission and machine learning — •Viktoriia Nikonova[1], Denys Kononenko[1], Dmitry Chernyavsky[1], Mikhail Seleznev[2], and Jeroen van den Brink[1,3] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, 01069 Dresden, Germany — [2]Institute of Materials Engineering, Technische Universitaet Bergakademie Freiberg, Gustav-Zeuner-Straße 5, D-09599, Freiberg, Germany — [3]Institute for Theoretical Physics, TU Dresden, 01069 Dresden, Germany

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