

## MM 10: Poster Session 1

Time: Monday 18:00–20:00

Location: P2

MM 10.1 Mon 18:00 P2

**Training Gaussian Approximation Potentials for Aqueous Systems** — ●NIKHIL BAPAT, MARTIN VONDRÁK, JOHANNES T. MARGRAF, HENDRIK H. HEENEN, and KARSTEN REUTER — Fritz-Haber-Institut der MPG, Berlin, Germany

An accurate and efficient description of aqueous systems via atomistic computer simulations is of high relevance for many applications. Machine learning potentials (MLPs) trained on first principles data have demonstrated promising accuracy and computational efficiency for the length and time scales critical to the description of water. But even with the compelling advancements in MLPs, building a successful data-efficient atomistic model for complex aqueous systems remains a challenging task. The training of such MLPs can be notoriously difficult and so far required either negligence of chemical reactivity in the MLP or excessive amounts of training data.

In this work we propose an efficient training procedure specifically designed for aqueous systems. To that end, we employ the widely applicable Gaussian approximation potential MLP and leverage it with a workflow for generating training data which ensures systematic inclusion of the bulk water configuration space. We calculate and compare ensemble properties of bulk water like its equilibrium density and diffusion coefficient to validate the MLP. The resulting model, when coupled with an added stimuli from a solid surface, can provide insights into many technologically important solid-liquid systems which are difficult to simulate otherwise.

MM 10.2 Mon 18:00 P2

**Transfer learning on organic/inorganic interfaces for different substrates** — ●ELIAS FÖSLEITNER, JOHANNES CARTUS, LUKAS HÖRMANN, and OLIVER T. HOFMANN — Graz University of Technology, Graz, Austria

Performing structure search of organic molecules on metallic surfaces requires finding the structure with the lowest energy. Using conventional density functional codes this proves to be a time-consuming task, since the number of possible configurations is large and individual calculations are expensive. For all-electron approaches, this becomes even more problematic when calculating molecules on metal substrates of higher nuclear charge number, e.g. on gold. To circumvent the computation of all possible configurations, machine learning techniques such as Gaussian process regression proved to be a useful tool to reduce the amount of calculated data.

In our work we further reduce the data requirements by using transfer learning from one substrate to another. To this end, we first train the system on substrate A, and use this information to accelerate the learning process of the system on another substrate B. This is done by using the energy predictions of substrate A as a prior for the machine learning model imposed on system B. By doing so, we can reduce the data requirements for the training of expensive systems to an extent that makes the investigation computationally feasible.

MM 10.3 Mon 18:00 P2

**Large-scale molecular dynamics simulations using fourth generation neural network potentials** — ●EMIR KOCER<sup>1</sup>, ANDREAS SINGRABER<sup>2</sup>, TSZ WAI KO<sup>1</sup>, JONAS FINKLER<sup>3</sup>, PHILIPP MISOF<sup>2</sup>, CHRISTOPH DELLAGO<sup>2</sup>, and JÖRG BEHLER<sup>1</sup> — <sup>1</sup>Georg-August University, Göttingen, Germany — <sup>2</sup>University of Wien, Vienna, Austria — <sup>3</sup>University of Basel, Basel, Switzerland

In the last decade, their proven success in bridging the gap between ab initio and classical molecular dynamics made machine learning potentials (MLP) very attractive. However, many MLPs are short-ranged and unable to capture interactions beyond a certain cutoff, which leads to inaccurate forces and energies in systems where long-range interactions are important. While MLPs including long-range electrostatic interactions based on local charges have been available for some years, only recently fourth generation MLPs have emerged that can take also global phenomena like non-local charge transfer into account. An example is the fourth generation high dimensional neural network potential (4G-HDNNP), which utilizes a global charge equilibration step. This study presents a modified version of 4G-HDNNPs, in which the matrix solution is replaced by a function minimization algorithm for an enhanced scalability on multi-core systems. The new potential has been implemented into the LAMMPS software and tested in large-scale

molecular dynamics simulations.

MM 10.4 Mon 18:00 P2

**Interatomic Potential Fitting in pyiron** — ●MARVIN POUL<sup>1</sup>, NIKLAS LEIMEROOTH<sup>2</sup>, ALEXANDER KNOLL<sup>3</sup>, MARIUS HERBOLD<sup>3</sup>, and JOERG NEUGEBAUER<sup>1</sup> — <sup>1</sup>Max-Planck-Institut fuer Eisenforschung — <sup>2</sup>Universitaet Goettingen — <sup>3</sup>TU Darmstadt

Interatomic potentials have a key role in computational materials science bridging the gap between Ab-Initio methods and large-scale engineering applications. pyiron[1] is an IDE for computational materials science that allows for reproducible yet easy to write simulation protocols. Within its framework we have developed tools that allow for semi-automatic fitting and verifying of potentials. This includes wrappers for AtomicRex[2] (for classical potentials) and as well the machine-learned Moment Tensor Potentials (MTP[3]), high-dimensional neural network potentials (HDNNP[4]), and ACE potentials. In this work we introduce the facilities offered by our code on the examples of an Magnesium MTP and an EAM potential for Copper.

[1]: <https://doi.org/10.1016/j.commatsci.2018.07.043>[2]: <https://doi.org/10.1088/1361-651X/aa6ecf>[3]: <https://doi.org/10.1088/2632-2153/abc9fe>[4]: <https://doi.org/10.1103/PhysRevLett.98.146401>

MM 10.5 Mon 18:00 P2

**Effect of temperature pre-treatments on atomic dynamics in PdNiP studied with ECM** — ●OLIVIA VAERST, MARTIN PETERLECHNER, and GERHARD WILDE — Institute of Material Physics, University of Münster, Germany

Pre-treatments on amorphous PdNiP, such as annealing and treatments of thermo-mechanical kind, significantly influence the local structure, kinetic stability, and mechanical properties of this bulk metallic glass (BMG).

In the present work, Pd<sub>40</sub>Ni<sub>40</sub>P<sub>20</sub> samples are pre-treated thermally by annealing them at different temperatures below the glass transition temperature. The resulting well-defined states are investigated via transmission electron microscopy (TEM) with electron correlation microscopy (ECM) at room temperature. ECM is used to study atomic rearrangements and dynamics in the material at nanometer spatial resolution [1,2]. The effect of thermal pre-treatments on ECM evaluation parameters is discussed. Such investigations of the atomic mobility in pre-treated PdNiP give further insight into underlying mechanisms and properties of the amorphous phase as well as on the local relaxation dynamics of a bulk metallic glass.

[1] L. He at al., *Microsc. and Microanal.* 21 (2015) 1026-1033.[2] K. Spangenberg et al., *Adv. Funct. Mater.* 31 (2021) 2103742.

MM 10.6 Mon 18:00 P2

**Investigating the short-range order of amorphous GeTe upon structural relaxation obtained by TEM diffractometry and RMC methods** — ●CHRISTIAN STENZ<sup>1</sup>, JULIAN PRIES<sup>1</sup>, T. WESLEY SURTA<sup>2</sup>, MICHAEL W. GAULTOIS<sup>2</sup>, and MATTHIAS WUTTIG<sup>1</sup> — <sup>1</sup>Institute of Physics IA, RWTH Aachen University, 52074 Aachen, Germany. — <sup>2</sup>Faculty of Chemistry, University of Liverpool, Liverpool L7 3NY, United Kingdom.

New experimental insights into the structural changes during resistance drift in amorphous GeTe are presented. Selected area electron diffraction is performed on a-GeTe in five different annealing states to compute the pair distribution functions upon relaxation. Examination of the short-range order based on the order parameters  $S(q_2)/S(q_1)$  and  $r_2/r_1$  implies a continuous increase in the most prominent average bond angle by  $1^\circ$  towards  $104.5^\circ$ . This is consistent with the analysis of the bond angle distribution (RMC simulations) which reveals a shift of the main contribution ( $\sim 103.5^\circ$ ) towards larger angles. A concomitant increase of intermediate geometries between tetrah. and octah. ( $\sim 140^\circ$ ) is observed. Applying three different techniques to estimate the fraction of tetrahedral Ge atoms the three measures coherently suggest a decrease in tetrahedrality. We conclude that an enhancement of Peierls-like distorted/pyramidal motifs, *i.e.* an increase in the  $PD$ -ratio  $r_L/r_S$ , causes the increase of the average bond angle, resulting in a widening of the band gap. This structural relaxation ultimately leads to the resistance drift.

MM 10.7 Mon 18:00 P2

**Influence of swift heavy ion irradiation on Pd-based metallic glasses** — ●SABA KHADEMORZAIAN<sup>1</sup>, MAXIMILLIAN DEMMING<sup>1</sup>, MARILENA TOMUT<sup>1,2</sup>, SERGIY DIVINSKI<sup>1</sup>, and GERHARD WILDE<sup>1</sup> — <sup>1</sup>Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — <sup>2</sup>GSI Helmholtzzentrum für Schwerionenforschung, 64291 Darmstadt, Germany

Bulk and ribbon samples of Pd<sub>40</sub>Ni<sub>40</sub>P<sub>20</sub> in as-quenched and relaxed states were room-temperature irradiated with 4.8 MeV/u 179Au ions at the UNILAC accelerator. Ion beam-induced surface patterning associated with irradiation masks and smoothening of the surface were studied by laser scanning microscope and profilometry. Irradiation induces an out-of-plane swelling step of approximately 100 nm as measured at the boundary between the irradiated and non-irradiated areas and can be explained by additional free volume creation in the solidified ion tracks. The swelling and plastic flow mechanisms are analyzed. Changes in the relaxation enthalpy have been investigated using differential scanning calorimetry. Low-temperature heat capacity measurements substantiate prominent irradiation-induced changes of the Boson peak. Furthermore, changes in diffusivity with increasing fluence was found by post-irradiation tracer diffusion measurements. The evolution of mechanical properties was probed by nanoindentation measurements and the changes induced by irradiation are compared with those caused by mechanical rejuvenation.

MM 10.8 Mon 18:00 P2

**Investigations on the relaxation of metallic glasses using fast scanning calorimetry** — ●MAXIMILIAN DEMMING, MARK STRINGE, MARTIN PETERLECHNER, and GERHARD WILDE — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, 48149 Münster

During isothermal annealing below the glass transition, all glasses, and thus also metallic glasses, show relaxation effects that resemble the underlying trajectory in phase space towards metastable equilibrium. Using fast scanning calorimetry (FSC) it becomes feasible to investigate such phenomena over a wide range of rates and at very high controlled heating or cooling rates. The tremendous advantage of FSC in comparison to a conventional differential scanning calorimeter (DSC) is, that here one can reach cooling and heating rates up to several 10000 K/s, which makes in-situ quenching possible. Another advantage is that a large number of measurements can be performed in small time intervals. This makes the FSC quite interesting for experiments in thermic cycling with controlled heating and cooling rates. One special method is the so-called cryogenic cycling, which means, that a sample is periodically quenched and reheated between room and a cryogenic temperature. According to literature, this treatment, that has been termed as \*cryogenic rejuvenation\* could lead to markedly changed properties of the metallic glass. The materials investigated here are AuCuSiAg and PdNiS due to their low glass transition temperature and melting point. In this work different relaxation states achieved by in-situ quenching via FSC are examined and compared to the relaxation behavior observed at conventional rates.

MM 10.9 Mon 18:00 P2

**Investigation of thermoelectric transport through infrared spectroscopy of Heusler and Heusler-like compounds based on Fe<sub>2</sub>VAl** — ●SAHRA BLACK, MICHAEL PARZER, FABIAN GARMROUDI, ERNST BAUER, ANDREI PIMENOV, and EVAN CONSTABLE — Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria

Thermoelectric materials have attracted much interest in recent years for their ability to convert a thermal gradient into an electric current, thereby acting as an electric power generator. Full and half Heusler compounds have attracted special interest in the growing field of thermoelectricity for several members with a high thermoelectric performance. One Heusler compound in particular Fe<sub>2</sub>VAl was under investigation for its high power Factor  $PF$  and its high thermoelectric figure of merit  $ZT$ . And recently the element doped thin film Fe<sub>2</sub>V<sub>0.8</sub>W<sub>0.2</sub>Al broke the world record for the highest thermoelectric figure of merit of roughly 5 ever recorded.

The purpose of the project was to investigate the dielectric response of the thermoelectric material class Fe<sub>2</sub>VAl under different manufacturing methods with the usage of Fourier-transformed infrared (FTIR) spectroscopy. This led to a better understanding of the different contribution to the thermoelectric figure of merit  $ZT$ .

MM 10.10 Mon 18:00 P2

**Atom probe tomography study of diffusion in Al-TiB<sub>2</sub> and Al<sub>3</sub>Ta-TiB<sub>2</sub> systems** — ●EVGENIYA VOLOBUEVA, PATRICK STENDER, JIEHUA LI, and GUIDO SCHMITZ — University of Stuttgart, Institute of Material Science, Heisenbergstr. 3, 70569, Stuttgart, Germany

To improve the quality of castings, grain refinement is a technique that can improve the overall qualities and properties of the material. For grain refinement in aluminum casting processes, TiB<sub>2</sub> and Ta are added. It is well known, that Al and Ta form an Al<sub>3</sub>Ta phase inside the Al-based alloy. In order to gain insight into the process of grain refinement, the diffusion of Al<sub>3</sub>Ta and Al in TiB<sub>2</sub> crystals was analyzed via Atom Probe Tomography (APT) in detail.

In this project, single crystals of TiB<sub>2</sub> were used as raw material, glued on top of tungsten posts. Both pure aluminum layers and stoichiometric Al<sub>3</sub>Ta layers were deposited by sputter deposition on these crystals with a layer thickness of 200 nm. Subsequent annealing treatments were carried out to investigate segregation and diffusion phenomena at the crystal interface. To use the high spatial and chemical resolution of APT, the samples were sharpened to a final apex radius of 50 nm by azimuthal milling using a Focused Ion Beam Instrument (FIB). Observed segregation and determined diffusion coefficients will be presented.

MM 10.11 Mon 18:00 P2

**Highly conductive Graphite Intercalated Compounds** — ●LEONHARD NIEMANN — Robert Bosch GmbH

Since its discovery, graphene has been a material of great research interest due to its promising properties of high electron mobility and electrical conductivity. However, the proposed applications have not yet been realized due to the complexity of fabricating high-quality, defect-free, large-area graphene films. Graphite, which consists of stacked graphene layers, does not have the same promising properties but is easier to fabricate. By intercalating Lewis acids between the graphene layers of graphite, the layers decouple and graphene like behaviour is achieved. The conductivity of these graphite intercalated compounds (GIC) is increased. Here, we report a gas-phase intercalation method for graphite films with AlCl<sub>3</sub>, resulting in GICs with 20 MS/m. These films exhibit good long-term thermal stability. It is noted that the final conductivity depends on the electrical conductivity of the untreated graphite films which is affected by defects in single graphene flakes and the flake size. Studies to increase the conductivity of non-intercalated graphite films are necessary to increase the conductivity of GICs. Therefore, further studies on graphenization of graphite films and defect healing are conducted and the results are presented.

MM 10.12 Mon 18:00 P2

**Flatbands and Nonlinear Transport in Nodal Line Semimetals** — ●THOMAS BÖMERICH, JINHONG PARK, and ACHIM ROSCH — Institute for Theoretical Physics, University of Cologne, Germany

Ohm's law describes the linear dependence of the current on the electric field. Although deviations from this relation are quite small for usual metals we present a model of a semimetal with large non-ohmic conductivity. Motivated by recent experiments on ZrTe<sub>5</sub> we study a low-energy Hamiltonian consisting of a single Dirac point which gets deformed into a nodal line by mirror symmetry breaking. Upon Landau quantization a zero energy state for a wide range of momenta emerges. For small densities the lowest Landau level can be reached at feasible magnetic fields making it possible to investigate the properties of the flatband.

While flatbands have generated growing interest because of their large density of states and the importance of interactions, we instead focus on their impact on nonlinear transport. Using the Boltzmann equation we obtain higher order conductivities and compare our results to a Dirac semimetal. We show that in the quantum limit, the nonlinear signal of the nodal line semimetal is five orders of magnitude larger than the Dirac semimetal. This enhancement of the nonlinear properties originates from the emergence of the flat bands in the nodal line semimetal. Additionally we investigate the influence of disorder on the linear conductivity.

MM 10.13 Mon 18:00 P2

**Towards an efficient formalism to calculate Electron-Phonon-coupling Self Energies and Transport properties from MD Simulation** — ●MARKUS KREMER<sup>1,2</sup>, MICHAEL CZERNER<sup>1,2</sup>, and CHRISTIAN HEILIGER<sup>1,2</sup> — <sup>1</sup>Institut für Theoretische Physik, Heinrich-Buff-Ring 16, 35392 Gießen, Germany — <sup>2</sup>Zentrum für Materialforschung Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

Calculating transport properties for finite temperature systems has been a concern of research for a long time, with the semiclassical Lowest-order-variational approximation to the Boltzmann-equation (LOVA) being the most commonly used. Recently it was presented that within the KKR formalism more accurate results can be obtained for some materials by using a quantum mechanical Landauer-Büttiker approach incorporating phase-breaking scattering.

Here we want to investigate the possibility of obtaining transport properties at finite temperatures by using a classical MD Simulation and carrying out a transport calculation in the KKR formalism of a certain amount of randomly picked MD screenshots. This procedure is repeated for different lengths of the device to verify that the cell shows ohmic behaviour and obtain its specific resistance. Afterwards we can map this specific resistance to a self-energy.

MM 10.14 Mon 18:00 P2

**Determination of interdiffusion coefficients for Pt-Pd binary system by Atom Probe Tomography and DFT calculations** — ●YOONHEE LEE<sup>1</sup>, XI ZHANG<sup>2</sup>, SEBASTIAN MANUEL EICH<sup>1</sup>, PATRICK STENDER<sup>1</sup>, BLAZEJ GRABOWSKI<sup>2</sup>, and GUIDO SCHMITZ<sup>1</sup> —

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Understanding the diffusion behavior of different alloy components is fundamental and many systems are well evaluated with distinct diffusivities. However, despite its significant usage as a catalyst for many applications, the interdiffusion behavior of the Pt-Pd binary system has not yet been fully uncovered due to the remarkably slow atomic migration. In this work, interdiffusion coefficients have been determined from experimental data and compared with the results of DFT simulations. For the temperature range between 400 and 700 °C, nano-sized multilayer samples were created by Ion-Beam Sputtering (IBS). After heat treatment, the samples are analyzed by Atom Probe Tomography (APT). Obtained composition profiles are fitted by a Fourier series approach and the respective interdiffusion coefficients are determined. For the temperature range between 800 and 970 °C, micron-sized Pt/Pd diffusion couples are used and analyzed using EDX. The respective interdiffusion coefficients are determined by the Boltzmann-Matano method. All interdiffusion coefficients are compared with DFT simulations.

MM 10.15 Mon 18:00 P2

**Imbibition- and Drying-Induced deformation of Nanoporous Solids** — ●JUAN SANCHEZ<sup>1</sup>, PATRICK HUBER<sup>1</sup>, HOWARD STONE<sup>2</sup>, LARS DAMMANN<sup>1</sup>, and ZHUOQUING LI<sup>1</sup> — <sup>1</sup>Hamburg University of Technology (TUHH), Hamburg, Germany — <sup>2</sup>Princeton University, NJ, USA

We present time-dependent macroscopic dilatometry experiments on the deformation of nanoporous monoliths (Vycor glass) upon spontaneous, capillarity-driven infiltration of water as well as drying. We find two distinct dynamical regimes. One of them can be quantitatively traced to deformation originating in changes in the surface stress at the inner pore walls (dynamic Bingham's regime), whereas the second results from Laplace pressure effects. The interplay of both strain-inducing regimes allows to infer the water content in the pore space.

The theoretical framework used to describe our experimental data combines simple continuum mechanics and fluid dynamics on the macroscopic porous-solid scale, supported by molecular dynamics simulations on the single-nanopore scale. Our study demonstrates that it is possible to monitor imbibition and drying dynamics by simple dilatometry measurements, offering multiple potential applications.

MM 10.16 Mon 18:00 P2

**The Interplay of Spreading, Imbibition and Evaporation of Droplets at Nanoporous Surfaces** — ●LAURA GALLARDO<sup>1,2,3</sup>, JUAN SANCHEZ<sup>1,2,3</sup>, OLIVIER VINCENT<sup>4</sup>, and PATRICK HUBER<sup>1,2,3</sup> —

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The dynamics of a droplet deposited on a porous substrate is a combination of three phenomena: spreading, imbibition and evaporation. Here we present a study on the interactions of droplets on nanoporous

silicon prepared by electrochemical etching as a function of time. The evolution of the droplet volume is analyzed theoretically and experimentally considering the evaporation and the imbibition of the liquid into the porous substrate. Water is employed to illustrate the case of an evaporation-dominated regime [1]. For an imbibition-dominated regime squalane is employed. The very low vapor pressure of this fluid allows for the analysis of the imbibition process of a droplet into a porous substrate without the contribution of evaporation. The agreement between the experimental data and the theoretical predictions deepens the understanding of the structure of HF-etched porous silicon substrates and provides new insights into the fundamentals of fluid transport in nanoporous media.

[1] Seker, Erkin, et al. APL 92.1 (2008): 013128

MM 10.17 Mon 18:00 P2

**Kinetic trapping in brittle crack opening** — ●TOBIAS MÜLLER and BERND MEYER — Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany

In the 1920s, Griffith introduced his continuum approach for fracture. Since then great efforts were made to describe crack propagation more precisely within continuum mechanics. Nevertheless, it is evident that the atomic structure of the crack tip itself plays a major role in crack advancement, thus making it necessary to extend the concept of Griffith to the discrete atomic level. This enables the possibility to investigate essential and material-specific processes, such as local bond rearrangements and path-dependent activation barriers. In general, crack opening is a complex chemical process on a multi-dimensional potential energy surface with many local minima and saddle points. The complexity even increases if parameters such as temperature, pressure or chemical environments are included. Here we discuss first DFT-based geometry optimizations for silicon to study brittle fracture mechanics. We show that cracks can propagate via a multitude of local energy minimum configurations connected by a variety of energy barriers. We highlight the complex nature of crack advancement and the complexity of modelling and finding the correct fracture pathway even for a material with a simple crystal structure such as silicon.

MM 10.18 Mon 18:00 P2

**Comparison of Crack - Dislocation Interactions in fcc and bcc Metals** — ●BENEDIKT EGGLE-SIEVERS and ERIK BITZEK — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf

The Interactions between Cracks and Dislocations are investigated by means of large scale atomistic simulations with EAM-potentials. Dislocations of different character and Burgers vector are placed in the vicinity of a strain-controlled crack, resulting either in an attraction or repulsion of the dislocation. In the former case further interactions can be observed in the course of the simulation, e.g. dislocation emission or crossslipping of screw parts. Dependencies on the stress state, the crack system, dislocation character and distance between dislocation and crack tip are investigated in fcc and bcc crystals. The results are discussed in the framework of resolved shear stresses acting on the dislocations in the near field of the crack tip and for different dislocations characteristics in fcc and bcc.

MM 10.19 Mon 18:00 P2

**Molecular dynamics analysis of point defects in ferroelectrics** — ●TAKAHIRO TSUZUKI<sup>1</sup>, DILSHOD DURDIEV<sup>2</sup>, FRANK WENDLER<sup>2</sup>, RYO KOBAYASHI<sup>1</sup>, MASAYUKI URANAGASE<sup>1</sup>, HIKARU AZUMA<sup>1</sup>, and SHUJI OGATA<sup>1</sup> — <sup>1</sup>Nagoya Institute of Technology, Nagoya, Japan — <sup>2</sup>Friedrich-Alexander University of Erlangen-Nürnberg, Fürth, Germany

Ferroelectrics are used in many devices such as capacitors. Pb(Zr, Ti)O<sub>3</sub> is the most used material in piezoelectric devices but it contains lead which is gradually prohibited using these days because lead is poisonous to human health. BaTiO<sub>3</sub>, which is a very famous classical ferroelectric and lead-free, is newly focused on because its characteristics improve treated by containing defects. But the mechanism of the effects of the defects is not well understood.

We investigated the effects of point defects, monovacancies, and first and second neighbor divacancies on the domain growth of BaTiO<sub>3</sub> with an applied electric field by molecular dynamics simulation using core-shell inter-atomic potential. We found that the first neighbor Ba-O divacancy is the most effective on the domain growth [1]. The sum of the electric field from the divacancy dipole and applied electric field, when they are in the same direction, strongly assist the domain growth.

Phase-field models are powerful tools to investigate ferroelectrics in

mesoscale simulation. We obtained parameters, which contain the effect of vacancies mentioned above, for a phase-field model from the molecular dynamics simulation.

[1] Tsuzuki T. et al., J. Appl. Phys. 131, 194101(2022).

MM 10.20 Mon 18:00 P2

**Effect of increasing Mn content on generalized planar fault energies of Ni-Mn-Ga alloys** — ●MARTIN HEČZKO<sup>1</sup>, PETR ŠESTÁK<sup>2</sup>, and MARTIN ZELENÝ<sup>1</sup> — <sup>1</sup>Institute of Materials Science and Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — <sup>2</sup>Institute of Physical Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic

Giant magnetic field induced strain (MFIS) in martensitic phase of Ni-Mn-Ga ferromagnetic shape memory alloy makes this alloy promising for various applications. The reasons for existence of MFIS are the high mobility of twin boundaries combined with large magneto-crystalline anisotropy. We performed our calculations using the spin-polarized DFT method implemented in the Vienna Ab Initio Simulation Package (VASP) to reveal the effect of increasing concentration of excess Mn on formation and propagation of twin boundaries, which can be characterized by changes in generalized planar fault energy (GPFE) curves. Effects of excess Mn local arrangement in Ga sublattice on GPFE curves has been considered as well.

Our results show that the barriers for nucleation and grow of a twin rise with increasing content of Mn. It results in more difficult twin formation and propagation in compositions far from stoichiometry. This effect is even more enhanced if excess Mn atom in Ga sublattice is located exactly in the planar fault.

MM 10.21 Mon 18:00 P2

**Influence of Twin Boundaries on the Mechanical Behavior of Nanowires Subjected to Bending** — ●SABA KHADIVIANAZAR<sup>1,2</sup>, JONAS SCHICKEL<sup>1</sup>, and ERIK BITZEK<sup>1,2</sup> — <sup>1</sup>Friedrich-Alexander-Universität Erlangen-Nürnberg, Chair of General Materials Properties, Institute I, Martensstr. 5, Erlangen 91058, Germany — <sup>2</sup>Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf 40237, Germany

Metallic nanowires (NWs) display superior mechanical properties compared to their bulk counterparts and are regarded as promising building blocks for a variety of application such as touchscreen displays, flexible and stretchable electronic devices. Recently it has been observed that the multi twinned nanowires show higher yield stress and enhanced localized deformation compared to the single crystalline nanowires. Despite the importance of characterizing the deformation behavior under bending loads, most studies of metallic twinned NWs to date have been performed under tensile testing conditions.

Here we present recent results of atomistic simulations on bi-crystalline twinned nanowires under bending. Atomistic simulations allow for controlled variation of the material, size, morphology, the location of the twin boundary (TB), and loading conditions. We show that the presence of a TB not only influences the plastic deformation but also affects the stress state of nanowires. The critical resolved shear stress for dislocation nucleation was determined and the interactions of dislocations with TBs was studied in detail for varying twin boundary location and bending directions.

MM 10.22 Mon 18:00 P2

**Benchmarking a Machine-Learning Enhanced Dimer Method for Transition State Search** — ●NILS GÖNNHEIMER, KING CHUN LAI, KARSTEN REUTER, and JOHANNES T. MARGRAF — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The implementation of Machine-Learning (ML) surrogate models into established atomistic simulation types (e.g. molecular dynamics or geometry optimizations) offers the opportunity of significantly lowering their computational cost. The Dimer method for finding saddle points on high-dimensional potential surfaces is a prime example of this. This method is an important tool for locating transition states and exploring reaction mechanisms in heterogeneous catalysis, but applications are limited by its large computational cost. Jacobsen et al. recently showed that this can be overcome by combining Dimer search with a Gaussian Process Regression surrogate model in the Artificial Intelligence-Driven dimer (AID-TS) algorithm. To better understand the role of the ML surrogate in this method, we compare accuracy, efficiency and diversity of the found states, for AID-TS and conventional dimer search, using surface self-diffusion of Pd(100) as an example.

MM 10.23 Mon 18:00 P2

**Al-Ge solid solubility prediction using machine-learned force-field potentials and phonon calculations** — ●ONDŘEJ FIKAR and MARTIN ZELENÝ — Institute of Materials Science and Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic

This work is focused on a theoretical study of the phase stability of Al rich solid solution in Al-Ge alloy. The solubilities of the solid solution were first determined using temperature-dependent free energies of pure elements and solid solutions of various chemical compositions obtained from ab initio calculations based on density functional theory. All total energy calculations were performed by Vienna Ab initio Simulation Package (VASP) with the help of Projector Augmented-wave potentials. Contributions of vibrational free energy and electron free energy were obtained from Phonopy package. Subsequently, a forcefield potential for Al-Ge alloy using machine learning routines as implemented in the VASP package was created. The trained forcefield potential was then used to again carry out phonon calculations. The results were compared to the previous phonon calculations carried out without machine learning.

MM 10.24 Mon 18:00 P2

**Simulation of long-term diffusion-based processes in Al and Ni** — ●DARIA SMIRNOVA<sup>1</sup> and ERIK BITZEK<sup>1,2</sup> — <sup>1</sup>Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — <sup>2</sup>Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

The study of coupled diffusive-displacive processes like dislocation climb at the atomic scale is inherently challenging due to the vastly different time scales involved in the individual processes. One way to address this challenge is to extend the possible simulation timescales while keeping proper atomistic description of a system by using diffusive molecular dynamics (DMD). The method combines classical atomistic interaction potentials in the variational Gaussian method with a numerical solver for the diffusion equation on a variable grid given by the atom positions. Recently, various computational implementations of DMD were presented. Here we describe in detail the different implementations of DMD and provide benchmarks for their efficiency using vacancy diffusion at defects in Al and Ni as model systems.

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**Ab initio study on novel precipitate-matrix interfaces in Al-Sc based alloys** — ●UJJAL SAIKIA<sup>1</sup>, TILMANN HICKEL<sup>1,2</sup>, SANKARAN SHANMUGAM<sup>3</sup>, SERGIY V. DIVINSKI<sup>4</sup>, and GERHARD WILDE<sup>4</sup> — <sup>1</sup>Department of Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH — <sup>2</sup>BAM Bundesanstalt für Materialforschung und -prüfung — <sup>3</sup>Indian Institute of Technology Madras — <sup>4</sup>Institute of Materials Physics, University of Münster

The cube-on-cube orientation relationship (OR) with the Al matrix has been accepted as the orientation relationship for the coherent nano-scaled Al<sub>3</sub>Sc-based particles in Al. Recently, in a severely cold-rolled and subsequently annealed Al-Sc-Zr-Ti alloy, atomic-scale investigations using high resolution scanning transmission electron microscopy (HRSTEM) reveals a novel type of precipitate/matrix coherency.

We performed density functional theory (DFT) based total energy calculations to understand the mechanism of formation of this new type of precipitate/matrix coherency between Al<sub>3</sub>Sc and Al matrix and to compare it with the established interfaces. Our DFT results reveal that the newly observed interface corresponds to a local minimum of energy and there is an energy penalty for the interface boundary to ‘escape’ the particle. We also studied segregation behavior of Sc atoms to probe the initial stage of formation of the observed novel Al<sub>3</sub>Sc/Al interface.

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**Ab initio study of point defects in disordered systems** — ●PAVEL PAPEZ<sup>1</sup>, MARTIN FRIÁK<sup>2</sup>, and MARTIN ZELENÝ<sup>1</sup> — <sup>1</sup>Institute of Materials Science and Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — <sup>2</sup>Institute of Physics of Materials, v.v.i., Czech Academy of Sciences, Brno, Czech Republic

This work is focused on a theoretical study of the influence of N and C interstitials in the equiatomic medium entropy alloy CoCrNi. These interstitials can be found in the alloy as contamination after preparation by powder-metallurgy techniques. The study was done by employing ab initio calculations based on the density functional theory and was performed by Vienna Ab initio Simulation Package (VASP)

using the projector-augmented-wave formalism. The calculations were done on  $6 \times 6 \times 2$  supercells generated by using the special quasi-random structures approach (SQS) consisting of 216 atoms. The supercell consisted of 6 lattice planes  $\{1\ 1\ 1\}$  along the  $z$ -axis. The hcp structures were made from the fcc cells by moving the planes to create the hcp ABABAB stacking. Our results have shown which interstitial positions result in the lower enthalpy of formation. They are characterized by a higher amount of Cr and lower amount of Ni in their nearest neighbours (NN) shell with the most stable being the one with 2 Co, 3 Cr, and 1 Ni in its 1st NN shell. The stacking fault energy (SFE) was calculated using the first-order axial Ising model and by explicit stacking-fault calculations in two times larger fcc supercell. The results shown that interstitials always increase the SFE.

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**Charge distribution and electronic structure of ZIF-8 and its derivatives from first principles** — •JOSHUA EDZARDS<sup>1</sup>, HOLGER-DIETRICH SASSNICK<sup>1</sup>, ANA MARIA VALENCIA<sup>1,2</sup> und CATERINA COCCHI<sup>1,2</sup> — <sup>1</sup>Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26129 Oldenburg — <sup>2</sup>Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin

Metal organic frameworks are novel materials with high potential in many fields of applications, ranging from gas storage and catalysis to optoelectronics. In spite of their growing popularity, there is still a lack of fundamental understanding of the physico-chemical properties of these materials, even in the most established subgroups such as the zeolitic imidazolate frameworks (ZIFs). To shed light into the nature of the chemical bonds in these systems, we performed a first-principles study based on density-functional theory investigating the charge distribution in ZIF-8 and its derivatives with Br, Cl, and H terminations replacing CH<sub>3</sub>. Our results indicate the presence of an ionic bond connecting the Zn atom to the organic scaffold, which is held together by covalent bonds. Control calculations performed on the building blocks of ZIF-8 indicate that the aforementioned characteristics are quantitatively influenced by the extended nature of the framework. The presence of halogen substituents, carrying around an excess of negative charge, leads only to a negligible redistribution of the charge density. On the other hand, the electronic structures computed for these systems indicate a reduction of about 0.5 eV of the band-gap in the Br- and Cl-terminated systems with respect to ZIF-8.

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**Recent progress in ICET** — J. MAGNUS RAHM, •ERIK FRANSSON, PERNILLA EKBORG-TANNER, JOAKIM BRORSSON, MATTIAS ÅNGQVIST, and PAUL ERHART — Department of Physics, Chalmers University of Technology, Gothenburg, Sweden

Alloy cluster expansions (CEs) provide an accurate and computationally efficient mapping of the potential energy surface of multi-component systems that enables comprehensive sampling of the many-dimensional configuration space. In this contribution, we provide an update regarding recent developments and new features in the integrated cluster expansion toolkit (ICET). We have implemented a version of the constituent strain formalism in ICET, which enables treatment of long-ranged strain contributions. This approach is demonstrated for the Pd-H system in order to study coherent phase transitions via constrained Monte Carlo simulations. Furthermore, in CEs of low-dimensional systems, lack of symmetry leads to large numbers

of independent effective cluster interactions (ECIs). We have made it possible to merge orbits, i.e., reduce the number of independent ECIs by considering local symmetries and merging parameters that are similar. This approach enables training of accurate models while requiring significantly fewer DFT calculations. This approach is employed to study surface segregation in AuPd and CuPd in environments ranging from vacuum to high pressures of hydrogen. Finally, we have added a number of additional features, including Wang-Landau sampling and extraction of long-range order parameters, and the code has undergone a thorough review that has resulted in a significant performance boost.

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**Molecular dynamics simulations of porous silica networks** — •HEMANGI PATEL<sup>1</sup>, BARBARA MILOW<sup>1,2</sup>, and AMEYA REGE<sup>1</sup> — <sup>1</sup>Institut für Werkstoff-Forschung, Abteilung Aerogele und Aerogelverbundwerkstoffe, Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR), Cologne, Germany — <sup>2</sup>Nanostructured Cellular Materials, Institut of Inorganic Chemistry, University of Cologne, Cologne, Germany

Molecular dynamics (MD) simulations offer a significant advantage over experimental procedures to investigate the nanoporous structure in silica-based systems because they present a detailed insight into the atomic-scale phenomena that underlie the formation of the materials\* network. In this work, porous silica networks are modelled using MD simulations.  $\alpha$ - quartz form of SiO<sub>2</sub> is subjected to high temperature and equilibration followed by quenching to obtain amorphous silica structure  $\alpha$ - quartz form of SiO<sub>2</sub> is subjected to high temperature and equilibration followed by quenching to obtain amorphous silica structure. The negative pressure rupturing approach is then used to obtain a fractal structure. Local minimum energy configuration is obtained using the conjugate gradient scheme for the formation of a stable porous network. The structural evolution of the silica backbone in the network is investigated. This technique is used to obtain porous networks of varying densities. The resulting model systems are investigated for their structural and mechanical properties. Uniaxial tensile and compressive simulations will be presented, and properties such as their Young's modulus will be quantified.

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**Magnetotransport properties of coupled nanowire arrays in LAO/STO** — •RANJANI RAMACHANDRAN<sup>1</sup>, DENG YU YANG<sup>1</sup>, MUQING YU<sup>1</sup>, ADITI NETHREWALA<sup>1</sup>, PATRICK IRVIN<sup>1</sup>, JEREMY LEVY<sup>1</sup>, and KI-TAE EOM<sup>2</sup> — <sup>1</sup>University of Pittsburgh, Pittsburgh, USA — <sup>2</sup>University of Wisconsin-Madison, Madison, WI, USA

The ability to create and characterise an array of coupled nanowires is an important step towards understanding the physics of systems like stripe phase superconductors, sliding Luttinger liquids, anisotropic materials made up of quasi-1D chains, etc. Here, we create nanowire arrays using Ultra Low voltage Electron beam lithography. ULVEBL has been shown to create conducting nanostructures in the 2D electron system at the LAO/STO interface. We study the transport properties of this system at low temperatures and high magnetic fields. We show that it is possible to reversibly tune the interwire coupling using a back gate voltage and magnetic field. This can act as a tool to study the dimensionality cross over from 1D to 2D. This can potentially be extended further to create more complicated structures using ULV-EBL that can model the behaviour of other materials and lattice models.