MM 37: Functional and Complex Materials

Time: Friday 12:00–12:45 Location: H22

MM 37.1 Fri 12:00 H22

Unveiling Material Dynamics with Machine-Learned Interatomic Potentials — •Ferenc Tasnadi, Bobur Mukhamedov, Amanda Ehn, Florian Trybel, and Igor A. Abrikosov — IFM Linköping University

Machine-learned interatomic potentials (MLIPs) have revolutionized our ability to understand the properties of materials with complex dynamical processes. In this work, we present an active learning MLIP strategy to: (i) investigate the elasticity of alloys near dynamical instability [1] and (ii) explore dynamical bond disorder in high-pressure synthesized PN2 [2]. bcc-Ti-based alloys have wide industrial applicability, ranging from low-modulus biomedical implants to high-strength GUM metals. The low-temperature dynamical instability of bcc-Ti can be tailored through the addition of bcc stabilizers (Nb, Ta, Zr, V), resulting in anomalous mechanical properties such as elinvar behavior or high anisotropy with low modulus in Ti-Nb-Zr and Ti-Zr-Sn alloys. Pnictogen compounds (Group 15 elements) exhibit fascinating chemistry due to the variety of bonding configurations, as demonstrated in the recently studied P-N system [2]. Long-timescale MLIP-driven simulations reveal that N-N distances connecting the P-N octahedra vary dynamically between single-bonded and non-bonding configurations. The results are compared with experimental observations. If time permits, we will demonstrate how MLIP-driven molecular dynamics simulations can offer deeper insights into materials exhibiting Peierls instability. [1] New J. Phys. 22 113005 (2020); J. Vac. Sci. Technol. A 42, 013412 (2024). [2] Chem. Eur. J. 2022, 28, e202201998.

MM 37.2 Fri 12:15 H22

Decoding Molecular Ion Dissociation Effects in Atom Probe Tomography of Iron Oxides — •Shyam Katnagallu[1], SeHo Kim[1], Shalini Bhatt[1], Daniel K Schreiber[2], Jörg Neugebauer[1], Baptiste Gault[1], and Christoph Freysoldt[1] — [1]Max Planck Institute for Sustainable Materials, Düsseldorf, Germany — [2]Energy and Environment Directorate, PNNL, Richland, USA.

To mitigate CO2 emissions, we require efficient carbon-free reduction processes for iron ores. Atom probe tomography (APT) can elucidate the gradual reduction of FexO at the nanometer length scale, but it is hindered by compositional bias. We investigated the changes in the measured composition of FeO, Fe2O3, and Fe3O4 across a range of analysis conditions. However, APT of ionic or covalently bonded materials often results in molecular ions. The metastability of these molecular ions, under an intense electrostatic field, makes them vulnerable to dissociation. These processes can significantly impact the analytical performance of APT. For instance, neutral molecules formed through dissociation may not be detected or may have a time-of-flight no longer associated with their actual mass, leading to their loss from the analysis. To predict possible dissociation reactions of molecular ions, we employed density-functional theory that considered the spin states of the molecules. The energetically favoured reactions were traced onto multi-hit correlation histograms to validate their existence within APT data. These detected reactions were carefully analysed to assess the impact of neutrals resulting from dissociation reactions on the performance of APT for analysing iron oxides.

MM 37.3 Fri 12:30 H22

Entropy Decoupling in Vacancy Formation of BCC High-Entropy Alloys — •Xiang Xu, Xi Zhang, and Blazej Grabowski — University of Stuttgart, Stuttgart, Germany

The temperature-dependent vacancy formation energies in MoTaNbW systems have been calculated using a machine-learning-based interatomic potential that accurately captures the simultaneous effects of configurational and vibrational entropies, along with their coupling. Our results indicate that at elevated temperatures, careful treatment of the chemical potential is essential. We computed the distributions of vacancy formation energies up to the melting point, explicitly accounting for anharmonic vibrational effects. The findings demonstrate that, in this system, the local atomic environment around a vacancy exerts minimal influence on the vibrational entropy contributions.