

MM 37: Transport in Materials: Diffusion, Conduction of Charge or Heat IV

Time: Wednesday 11:45–12:45

Location: C 264

MM 37.1 Wed 11:45 C 264

Atomistic modelling of bulk and grain boundary diffusion for solid electrolyte $\text{Li}_6\text{PS}_5\text{Cl}$ — •YONGLIANG OU¹, YUJI IKEDA¹, SERGIY DIVINSKI², and BLAZEJ GRABOWSKI¹ — ¹Institute for Materials Science, University of Stuttgart, 70569 Stuttgart, Germany — ²Institute of Materials Physics, University of Münster, 48149 Münster, Germany

$\text{Li}_6\text{PS}_5\text{Cl}$ is a promising candidate for the solid electrolyte in all-solid-state Li-ion batteries. In applications, this material exists in a polycrystalline state with many grain boundaries (GBs) rather than a single-crystalline state. Atomistic modeling of $\text{Li}_6\text{PS}_5\text{Cl}$ with GBs, however, remains rare due to high computational cost. Here, machine-learning interatomic potentials, specifically moment tensor potentials (MTPs), are employed to accelerate simulations while preserving the *ab initio* accuracy. Two tilt GBs $\Sigma 3(1\bar{1}2)[110]$, $\Sigma 3(\bar{1}11)[110]$ and one twist GB $\Sigma 5(001)[001]$ are investigated, all of which exhibit low GB energies based on the annealing and quenching relaxation approach. Diffusion coefficients are calculated through mean square displacements obtained by molecular dynamics simulations. Enhanced Li diffusion compared to the perfect bulk is observed at GBs. A connection between GB morphology and its effects on Li diffusion is revealed, paving the way for improved solid electrolyte design through GB engineering.

MM 37.2 Wed 12:00 C 264

Navigating the Interface: Exploring Grain Boundaries in Solid-State Electrolytes through Ultrafast Interpretable ML Potentials — •TABEA HUSS, CARSTEN G. STAACKE, KARSTEN REUTER, and CHRISTOPH SCHEURER — Fritz-Haber-Institut der MPG, Berlin

The lithium thiophosphate (LPS) material class provides promising candidates for solid-state electrolytes (SSE) in lithium ion batteries due to high lithium ion conductivities and low material cost. The most performant glass-ceramic SSEs from the LPS class are characterized by omnipresent two-dimensional interfaces between crystalline and glassy domains, which can dominate the material performance and cycle stability.

Atomistic simulations are challenged by the complexity of these grain boundaries, having to both capture the complex chemistry of these materials and their low degree of order. Here, we tackle this with newly introduced ultra-fast interpretable machine learning potentials (UFP)[1] to combine the high accuracy of machine learned potentials with the speed of classical ones. This enables us to explore polycrystalline solid-solid interfaces within the LPS system on a grand scale, encompassing system sizes exceeding 10,000 atoms and time scales

spanning multiple nanoseconds across substantial ensemble sizes. Ultimately we conduct a comprehensive analysis of grain boundaries in LPS aiming to understand their stability and their influence on the transport of lithium ions.

[1] S. R. Xie et al., npj Comp. Mater. 9, 162 (2023).

MM 37.3 Wed 12:15 C 264

Grain boundary diffusion of 57Co in Cu SIGMA-5 (310) bicrystals — •ESAKKIRAJA NEELAMEGAN¹, DANIEL GAERTNER¹, HUI DING², ANOOSHEH AKBARI¹, CHRISTIAN H LIEBSCHER², GERHARD WILDE¹, and SERGIY V DIVINSKI¹ — ¹Institute of Materials Physics, University of Münster, Münster, 48149 Germany — ²Structure and Nano- / Micromechanics of Materials, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Diffusion of 57Co in pure copper SIGMA-5(310)[001] bicrystals is investigated using the radiotracer technique. The measurements are performed both in type B (> 950 K) and type C (< 850 K) kinetics regimes after Harrison classification. The tracer diffusion experiments are conducted by varying the amount of the applied 57Co tracer solution, and the characteristic changes in the shape of the penetration profiles are related to the Co segregation-induced changes of the grain boundary structure.

MM 37.4 Wed 12:30 C 264

Grain- and phase boundary diffusion in AlCoCrFeNi2.1 compositionally complex alloy — •HENG ZHANG, MOHAN MURALIKRISHNA, SERGIY DIVINSKI, and GERHARD WILDE — Institute of Materials Physics, University of Muenster, Wilhelm-Klemm-Str. 10, 48149, Muenster

Grain and phase boundary diffusion of 63Ni is investigated in a Al-Co-Cr-Fe-Ni multi-principal element system. For better understanding on the influence of chemical complexity and the crystal structure on the atomic transport, Ni diffusion is systematically measured in two-phase (FCC+B2) eutectic AlCoCrFeNi2.1 alloy and its single phase FCC and B2 counterparts. Grain boundary (GB) diffusion of Ni is found to be similar in all three alloys substantiating enhanced phase boundary diffusion in the eutectic alloy on par with GB diffusion in single phase alloys. However, when compared on the homologous scale, GB diffusion in FCC and eutectic alloys is found to be similar and it is faster in the single phase B2 HEA. The measured GB diffusivities are compared with the GB self-diffusion rates in pure elements and alloys. An impact of chemical complexity on grain and phase boundary diffusion is discussed in terms of the *sluggish* diffusion concept invented for the high-entropy alloys.