Breakout Session: Interfaces (solid/liquid)

Jeffery A. Greathouse

Sandia National Laboratories
Albuquerque, New Mexico

5th LAMMPS Workshop and Symposium
August 2017 - Albuquerque, NM

Sandia National Laboratories

System details

Sandia National Laboratories

Types of interfaces

- Solid-gas
- Solid-Solid
- Liquid-Gas
- Liquid-Liquid
- **Solid-Liquid**

Properties to be simulated

- Structure
- Transport
- Spectroscopic

Interaction potentials

- Atomistic
- Coarse-grained
- Same pair style for both phases (hopefully)
- Hybrid pair style

LAMMPS resources for interfaces

Sandia National Laboratories

See breakout resource pages for solid-state and soft matter

Pair styles

- pair hybrid
- pair hybrid/overlay

Solid-state pair styles

- pairwise: born, buckingham, morse
- many-body: eam, edip, eim, gw, mgpt, sw, terso, meam, nb3b, polymorphic, rebo, airebo, snap, sw, terso,vashishita
- reactive: comb, comb3, reax/c (omp,kokkos)
- kim = https://openkim.orgpair hybrid/overlay

Soft matter pair styles

- pair: morse, charmm, class2, lj/coul, nm, tip4p
- reactive: reax/c (omp,kokkos)
- kim = https://openkim.org

Pre- and post-processing

Sandia National Laboratories

Pre-processing

- Initial configuration
- Choice of FF, boundary conditions
- Solid phase – fixed atoms or mobile/flexible

Post-processing

- Not the same as bulk phases
- Calculation of properties as a function of distance from the interface