Breakout session: Solid-state materials

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LAMMPS resources for solid-state materials

- Manual
  - Section 6.12 = orthogonal vs triclinic
  - Section 6.18 = elastic constants
  - Section 6.20 = thermal conductivity
  - Section 6.26 = core/shell model
- Commands
  - lattice = define crystal lattice params
  - create_atoms = create crystal lattice of atoms
  - change_box = orthogonal or triclinic boxes
- Pair styles
  - pairwise: born, buckingham, morse
  - many-body: eam, edip, eim, gw, meam, mgpt, nb3b, polymorphic, rebo, airebo, snap, sw, tersoff, vashishita
  - reactive: comb, comb3, reax/c (omp,kokkos)
  - kim = https://openkim.org

LAMMPS resources (continued)

- Fixes
  - box/relax, orient/bcc, orient/fcc, msst, neb, nphug, thermal/conductivity, ttm
- Computes
  - coord/atom, cna/atom, centro/atom, voronoi/atom, heat/flux, ackland/atom, xrd, basal/atom
- Packages
  - SHOCK, USER-SMD, USER-DIFFRACTION, CORESHELL, REPLICA, USER-PHONON
- Example dirs
  - comb, coreshell, crack, eim, friction, gcmc, hugoniostat, indent, meam, msst, nb3b, neb, peri, prd, streitz, tad, vashishita, voronoi, KAPPA, ELASTIC, ELASTIC_T, HEAT
- Website: Offsite tools (JAZZ)