Embedded-atom potential for cobalt published in


The potential files were originally generated in the input format of the SOLD code, and were later converted to the eam.alloy format of LAMMPS. To check the accuracy of the conversion, the following properties of Co were computed with both SOLD and LAMMPS: cohesive energy EcOh and lattice constants a and c for the HCP, FCC and BCC phases.

HCP-Co phase
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LAMMPS: EcOh = -4.3910543025 eV/atom; SOLD: EcOh = -4.3910550000 eV/atom
LAMMPS: a = 2.51866215 Å; SOLD: a = 2.51866155 Å
LAMMPS: c/a = 1.61025910; SOLD: c/a = 1.61025846

FCC phase
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LAMMPS: EcOh = -4.3848785080625 eV/atom;
SOLD: EcOh = -4.3848789062500 eV/atom
LAMMPS: a = 3.5642219 Å; SOLD: a = 3.5642187 Å

BCC phase
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LAMMPS: EcOh = -4.3273334702125 eV/atom;
SOLD: EcOh = -4.3273330078125 eV/atom
LAMMPS: a = 2.8149854 Å; SOLD: a = 2.8149811 Å;