

Embedded-atom potential for cobalt published in

G.P. Purja Pun and Y. Mishin, Physical Review B, 86, 134116 (2012)

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 E_{coh} and lattice constants a and c for the HCP, FCC and BCC phases.

HCP-Co phase

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LAMMPS: $E_{coh} = -4.3910543025$ eV/atom; SOLD: $E_{coh} = -4.3910550000$ eV/atom

LAMMPS: $a = 2.51866215$ A; SOLD: $a = 2.51866155$ A

LAMMPS: $c/a = 1.61025910$; SOLD: $c/a = 1.61025846$

FCC phase

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LAMMPS: $E_{coh} = -4.3848785080625$ eV/atom;

SOLD: $E_{coh} = -4.3848789062500$ eV/atom

LAMMPS: $a = 3.5642219$ A; SOLD: $a = 3.5642187$ A

BCC phase

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LAMMPS: $E_{coh} = -4.3273334702125$ eV/atom;

SOLD: $E_{coh} = -4.3273330078125$ eV/atom

LAMMPS: $a = 2.8149854$ A; SOLD: $a = 2.8149811$ A;