Release notes

11 September 2013

Mishin-Al-Co-2013.eam.alloy (to be published)

This file and the interatomic potential can be found at http://www.ctcms.nist.gov/potentials/.

The following table shows results of assessment of accuracy of the conversion from the files in the 'plt' format to the setfl format (Mishin-Al-Co-2013.eam.alloy converted by G. P. Purja Pun on 11 September 2013). The conversion was done by interpolating the 'plt' files using cubic splines, ensuring $\rho(r)$ and $\phi(r)$ starts at $r = 0$.

Reference to pure Al: Y. Mishin, D. Farkas, M. J. Mehl and D. A. Papaconstantopoulos, Phys. Rev. B 59, 3393 (1999)

Reference to pure Co: G. P. Purja Pun and Y. Mishin, "Embedded-atom potential for hcp and fcc cobalt", Phys. Rev. B 86, 134116 (2012).

Comparison of energies (in ev/atom) from SOLD and LAMMPS:

Alloy	a (A)	E_{min}(SOLD)	E_{min}(LAMMPS)
fcc Al	4.0500009365231735003	-3.36000000	-3.35999999
hcp Co*	2.5068053489070201145	-4.39006850	-4.39006855
fcc Co	3.5642218359374711056	-4.38487891	-4.38487851
B2 AlCo	2.7967728906249997856	-4.51486414	-4.51486416
$L1_2$ Al_3Co	3.8597793750002056257	-3.61656719	-3.61656719

* c/a = 1.6329931618554520689