Release notes

11 September 2013

Mishin-Ni-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-Ni-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 Ni: Y. Mishin, Acta Mater. 52, 1451 (2004)

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 Ni	3.520000062500039828	-4.45000000	-4.44999998
hcp Co*	2.506804859296695831	-4.39006875	-4.39006855
fcc Co	3.5642218359374711056	-4.38487891	-4.38487851
B2 NiCo	2.9223666069595646277	-4.26841875	-4.26841872
$L1_2$ Ni_3Co	3.6092475000000070473	-4.43114023	-4.43114005

* c/a = 1.6329931618554518469