Release notes

11 September 2013

Mishin-Ni-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-Ni-Al-Co-2013.eam.alloy converted by G. P. Purja Pun on 6 September 2013). The conversion was done by interpolating the 'plt' files using cubic splines, ensuring $\rho(r)$ and $\phi(r)$ starts at $r = 0$.

The original reference to the binary Ni-Al potential is: G. P. Purja Pun and Y. Mishin, "Development of an interatomic potential for the Ni-Al system", Phil. Mag. 89, 3245 (2009). The elemental Co potential is referred to G. P. Purja Pun and Y. Mishin, "Embedded-atom potential for hcp and fcc cobalt", Phys. Rev. B 86, 134116 (2012).

The remaining binary systems, Al-Co and Ni-Co, are to be published.

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
fcc Al	4.0500013332031115453	-3.36000000	-3.35999999
hcp Co*	2.506804859296695831	-4.39006875	-4.39006855
fcc Co	3.5642218359374711056	-4.38487891	-4.38487851
B2 NiAl	2.8319904492187424339	-4.51087101	-4.51087102
B2 NiCo	2.9223666069595646277	-4.26841875	-4.26841872
B2 AlCo	2.7967728906249997856	-4.51486414	-4.51486416
$L1_2$ Ni_3Al	3.5331693749999457665	-4.63147812	-4.63147796
$L1_2$ Al_3Co	3.8597793750002056257	-3.61656719	-3.61656719
$L1_2$ Ni_3Co	3.6092475000000070473	-4.43114023	-4.43114005
cF16 Al_2CoNi	5.7351898500000002556	-4.52657211	-4.52657213

* c/a = 1.6329931618554518469