

Ni99.eam.alloy release notes, 14 February 2009. This file and the interatomic potential can be found at <http://www.ctcms.nist.gov/potentials/>.

These are the results of tests done to assess the accuracy of the conversion from Yuri Mishin's Ni files in the x,y plt format to the setfl format (Ni99.eam.alloy, conversion 14 February 2009 by C.A. Becker). The conversion was done by interpolating the plt files using cubic splines, ensuring the rho(r) and phi(r) started at r=0. The converter is adapted from Yuri Mishin's SOLD (Simulator of Lattice Defects) program in order to be as consistent as possible with previous results. For all tests, the simulation contained 1 unit cell with atoms in their ideal positions. Conjugate gradient energy minimization was used to minimize the total energy. The SOLD program was kindly provided by Yuri Mishin.

The original reference for this potential is: Y. Mishin, D. Farkas, M.J. Mehl, and D.A. Papaconstantopoulos, "Interatomic potentials for monoatomic metals from experimental data and ab initio calculations," Phys. Rev. B 59, 3393 (1999).

To use the file Ni99.eam.alloy with LAMMPS, the following should be included in the input file:

```
units          metal
atom_style     atomic
pair_style     eam/alloy
pair_coeff     * * Ni99.eam.alloy Ni
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Comparison of minimum energies from SOLD and LAMMPS

Element	a (A)	E_min(SOLD,eV)	E_min(LAMMPS,eV)	Notes
fcc Ni	3.51	-0.177981969810E+02	-17.7981969809	
	3.52	-0.177999999941E+02	-17.7999999934	= -4.4499999975 eV/atom
	3.53	-0.177981918528E+02	-17.7981918528	

EAM function values from SOLD and LAMMPS

Ni a=3.52 A

r^2	rho(SOLD)	rho(LAMMPS)
6.195200	0.075149024627842	0.075149024628745
12.390400	0.009536003729777	0.009536003729777
18.585600	0.001655380098140	0.001655380098126
24.780800	0.000100234413743	0.000100234413743
30.976000	0.000002657455504	0.000002657455504

r^2	phi(SOLD)	phi(LAMMPS)
6.195200	-0.111392608782414	-0.111392608767647
12.390400	-0.015780833811480	-0.015780833811467
18.585600	-0.003023968758320	-0.003023968758305
24.780800	0.002049200952706	0.002049200952707
30.976000	0.000590864520833	0.000590864520834

rho(SOLD)	F(SOLD)
1.000000032165157	-2.984799600000084
1.000000032165158	-2.984799600000084
rho(LAMMPS)	F(LAMMPS)
1.000000032175635	-2.984799600000085