

Al03.eam.alloy release notes, 11 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 Al files in the x,y plt format to the setfl format (Al03.eam.alloy, conversion 4 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 periodic boundary conditions and 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: R.R. Zope and Y. Mishin, "Interatomic potentials for atomistic simulations of the Ti-Al system," Phys. Rev. B 68, 024102 (2003).

To use the file Al03.eam.alloy with LAMMPS, the following should be included in the input file:

```
units          metal
atom_style     atomic
pair_style     eam/alloy
pair_coeff     * * Al03.eam.alloy Al
```

Comparison of minimum energies from SOLD and LAMMPS

Element	a (A)	E_min(SOLD,eV)	E_min(LAMMPS,eV)	Notes
fcc Al	4.045	-0.134397744936E+02	-13.4397744936	= -3.360000023 eV/atom
	4.05	-0.134400000917E+02	-13.4400000916	
	4.055	-0.134397762952E+02	-13.4397762952	

EAM function values from SOLD and LAMMPS

Al a=4.05 A

r^2	rho(SOLD)	rho(LAMMPS)
8.201250	0.056304988380970	0.056304988380983
16.402500	0.026181183722012	0.026181183722155
24.603750	0.006599895956940	0.006599895956939
32.805000	0.000722317898493	0.000722317898493
41.006250	0.000007823399479	0.000007823399479

r^2	phi(SOLD)	phi(LAMMPS)
8.201250	-0.084616103339349	-0.084616103338304
16.402500	-0.008659701806386	-0.008659701806418
24.603750	0.012926429227054	0.012926429227056
32.805000	0.007417175893879	0.007417175893873
41.006250	0.000162983142243	0.000162983142242

rho(SOLD)	F(SOLD)
1.000000042239676	-2.695800579595233
rho(LAMMPS)	F(LAMMPS)
1.000000042240670	-2.695800579596680
1.000000042240669	-2.695800579596680