Al99.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 (Al99.eam.alloy, conversion 30 December 2008 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 Al99.eam.alloy with LAMMPS, the following should be included in the input file:

```
units          metal
atom_style     atomic
pair_style     eam/alloy
pair_coeff     * * Al99.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	-0.134397753172E+02	-13.4397753174	
	4.05	-0.134399999525E+02	-13.4399999525	= -3.359999988125 eV/atom
	4.055	-0.134397761746E+02	-13.4397761743	

EAM function values from SOLD and LAMMPS

Al a=4.05 A

r^2	rho(SOLD)	rho(LAMMPS)
8.201250	0.074118766034737	0.074118766040777
16.402500	0.008018049123605	0.008018049028526
24.603750	0.002288913416858	0.002288913416527
32.805000	0.000628309701782	0.000628309693000

r^2	phi(SOLD)	phi(LAMMPS)
8.201250	-0.021456387999719	-0.021456387999721
16.402500	-0.027491448591410	-0.027491448591413
24.603750	-0.010208454558396	-0.010208454558405
32.805000	0.001851934890693	0.001851934890694

rho(SOLD)	F(SOLD)
1.000007125584451	-2.714794949876448
rho(LAMMPS)	F(LAMMPS)
1.000007124973119	-2.714794949876463