Ag.eam.alloy release notes, 10 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 Ag files in the x,y plt format to the setfl format (Ag.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 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: P.L. Williams, Y. Mishin, and J.C. Hamilton, "An embedded-atom potential for the Cu-Ag system," Modelling Simul. Mater. Sci. Eng. 14, 817 (2006).

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

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

Comparison of minimum energies from SOLD and LAMMPS

Alloy	a (A)	E_min(SOLD,eV)	E_min(LAMMPS,eV)	Notes
fcc Ag	4.085	-0.113996999978E+02	-11.3996999978	
	4.09	-0.113999998989E+02	-11.3999998989	= -2.849999974725 eV/atom
	4.095	-0.113997024609E+02	-11.3997024609	

EAM function values from SOLD and LAMMPS

Ag a=4.09 A

r^2	rho(SOLD)	rho(LAMMPS)
8.364050	0.052809106347910	0.052809106347920
16.728100	0.005997594627096	0.005997594627097
25.092150	0.001015038036291	0.001015038036293
33.456200	0.000005644778750	0.000005644778750

r^2	phi(SOLD)	phi(LAMMPS)
8.364050	-0.069884871632783	-0.069884871632867
16.728100	-0.021820155137812	-0.021820155137818
25.092150	-0.004792825717495	-0.004792825717494
33.456200	-0.000029898340731	-0.000029898340730

rho(SOLD)	F(SOLD)
0.694123494153490	-1.765073986996962
rho(LAMMPS)	F(LAMMPS)
0.694123494153646	-1.765073986991016