Cu01.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 Cu files in the x,y plt format to the setfl format (Cu01.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: Y. Mishin, M.J. Mehl, D.A. Papaconstantopoulos, A.F. Voter, and J.D. Kress, "Structural stability and lattice defects in copper: Ab initio, tight-binding, and embedded-atom calculations," Phys. Rev. B, 63, 224106 (2001).

To use the file Cu01.eam.alloy with LAMMPS, the following should be included in the input file:

```
units          metal
atom_style     atomic
pair_style     eam/alloy
pair_coeff     * * Cu01.eam.alloy Cu
```

Comparison of minimum energies from SOLD and LAMMPS

Element	a (A)	E_min(SOLD,eV)	E_min(LAMMPS,eV)	Notes
fcc Cu	3.614	-0.141599858160E+02	-14.1599858159	
	3.615	-0.141599998733E+02	-14.1599998735	= -3.539999968 eV/atom
	3.616	-0.141599858326E+02	-14.1599858326	

EAM function values from SOLD and LAMMPS

Cu a=3.615 A

r^2	rho(SOLD)	rho(LAMMPS)
6.534113	0.074438078198329	0.074438078198329
13.068225	0.010584879936571	0.010584879936569
19.602338	0.001752795817922	0.001752795817922
26.136450	0.000097232932414	0.000097232932414

r^2	phi(SOLD)	phi(LAMMPS)
6.534113	-0.085917044257349	-0.085917044257347
13.068225	-0.025206079313094	-0.025206079313093
19.602338	-0.003383716205807	-0.003383716205807
26.136450	0.000483680216410	0.000483680216410

rho(SOLD)	F(SOLD)
1.000000112818476	-2.282353935027271
rho(LAMMPS)	F(LAMMPS)
1.000000112818457	-2.282353935071510
1.000000112818458	-2.282353935071510