CuAg.eam.alloy release notes, 6 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-Ag files in the x,y plt format to the setfl format (CuAg.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: 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 CuAg.eam.alloy with LAMMPS, the following should be included in the input file:

```
units          metal
atom_style     atomic
pair_style     eam/alloy
pair_coeff     * * CuAg.eam.alloy Cu 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	
fcc Cu	3.614	-0.141599858176E+02	-14.1599858176	
	3.615	-0.141599998746E+02	-14.1599998747	= -3.539999968675 eV/atom
	3.616	-0.141599858326E+02	-14.1599858326	
L12 Ag3Cu	3.9834	-0.117565455676E+02	-11.7565455676	
	3.9835	-0.117565455929E+02	-11.7565455929	= -2.939136398225 eV/atom
	3.9836	-0.117565453583E+02	-11.7565453583	
L10 CuAg	3.880	-0.123070560947E+02	-12.3070560948	
	3.881	-0.123070804962E+02	-12.3070804962	= -3.07677012405 eV/atom
	3.882	-0.123070738275E+02	-12.3070738275	
L12 Cu3Ag	3.757	-0.130877673407E+02	-13.0877673407	
	3.758	-0.130877880950E+02	-13.087788095	= -3.27194702375 eV/atom
	3.759	-0.130877780304E+02	-13.0877780304	

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

Cu a=3.615 A

r^2	rho(SOLD)	rho(LAMMPS)
6.534113	0.074438078197132	0.074438078197132
13.068225	0.010584879936254	0.010584879936254
19.602338	0.001752795817842	0.001752795817842
26.136450	0.000097232932393	0.000097232932393

r^2	phi(SOLD)	phi(LAMMPS)
6.534113	-0.085917094601247	-0.085917094601247
13.068225	-0.025206086470247	-0.025206086470246
19.602338	-0.003383717391191	-0.003383717391191
26.136450	0.000483680150608	0.000483680150609

rho(SOLD)	F(SOLD)
1.000000112800040	-2.282353259026427
1.000000112800041	-2.282353259026427
rho(LAMMPS)	F(SOLD)
1.000000112800027	-2.282353259069421
1.000000112800028	-2.282353259069421

Ag3Cu a=3.9835 A

r^2	rho(SOLD)	rho(LAMMPS)
7.934136	0.060448446232752	0.060448446232753
7.934136	0.047786975220585	0.047786975220593
15.868272	0.004873535457694	0.004873535457693
15.868272	0.007295173660020	0.007295173660018
23.802408	0.000446018874416	0.000446018874416
23.802408	0.001337948480224	0.001337948480224
31.736545	0.000055507232848	0.000055507232848

r^2	phi(SOLD)	phi(LAMMPS)
7.934136	-0.063405618491584	-0.063405618491312
7.934136	-0.066914517227865	-0.066914517227888
15.868272	-0.011843350853838	-0.011843350853838
15.868272	-0.025558143074423	-0.025558143074424
23.802408	-0.005584260361660	-0.005584260361652
23.802408	-0.006120633587666	-0.006120633587666
31.736545	-0.000292114577484	-0.000292114577484

rho(SOLD)	F(SOLD)
0.744147926177557	-1.761326155379545
0.744147926177558	-1.761326155379545
0.786733331064550	-2.241426154635603
rho(LAMMPS)	F(LAMMPS)
0.744147926177580	-1.761326155382139
0.786733331064559	-2.241426154635823

CuAg a=3.881 A

r^2	rho(SOLD)	rho(LAMMPS)
7.531080	0.068831525173082	0.068831525173080
7.531080	0.054186095600210	0.054186095600218

15.062161	0.006080456724170	0.006080456724169
15.062161	0.008803199186570	0.008803199186570
22.593241	0.000711470478117	0.000711470478117
22.593241	0.001720095287869	0.001720095287870
30.124322	0.000192620398659	0.000192620398659
30.124322	0.000000000230360	0.000000000230360

r^2	phi(SOLD)	phi(LAMMPS)
7.531080	-0.050945253729133	-0.050945253728880
7.531080	-0.062803207591688	-0.062803207591700
7.531080	-0.086380896229374	-0.086380896229291
15.062161	-0.014828002204525	-0.014828002204525
15.062161	-0.029658479061344	-0.029658479061339
22.593241	-0.000249681587347	-0.000249681587348
22.593241	-0.007619554463935	-0.007619554463949
22.593241	-0.007685846221929	-0.007685846221936
30.124322	-0.000997722247740	-0.000997722247740
30.124322	0.000000005114154	0.000000005114154

rho(SOLD)	F(SOLD)
0.789089795350161	-1.751991693015179
0.837092615325674	-2.259600173059315
rho(LAMMPS)	F(LAMMPS)
0.789089795350226	-1.751991693013199
0.837092615325693	-2.259600173059087

Cu3Ag a=3.758 A

r^2	rho(SOLD)	rho(LAMMPS)
7.061282	0.062852970138718	0.062852970138713
7.061282	0.080422918188860	0.080422918188852
14.122564	0.007884125490181	0.007884125490182
14.122564	0.011022393370322	0.011022393370319
21.183846	0.001113794054072	0.001113794054071
21.183846	0.002301934021530	0.002301934021529
28.245128	0.000004416130543	0.000004416130543
28.245128	0.000444063188335	0.000444063188335
35.306410	0.000000017231091	0.000000017231090

r^2	phi(SOLD)	phi(LAMMPS)
7.061282	-0.051746694850591	-0.051746694850604
7.061282	-0.088898522362072	-0.088898522362017
14.122564	-0.019108034575602	-0.019108034575602
14.122564	-0.035264699809090	-0.035264699809092
21.183846	-0.001446381632289	-0.001446381632290
21.183846	-0.010516854510566	-0.010516854510556
28.245128	0.000052252751389	0.000052252751390
28.245128	-0.002236685226569	-0.002236685226569
35.306410	-0.000000042896298	-0.000000042896298

rho(SOLD)	F(SOLD)
0.852429817444297	-1.730440623420056
0.908109495258908	-2.275710973226181
0.908109495258909	-2.275710973226181
rho(LAMMPS)	F(LAMMPS)
0.852429817444197	-1.730440623413965
0.908109495258811	-2.275710973226475