

Au-Grochola-JCP05.eam.alloy notes, 2 February 2011.

These are the results of tests done to assess the accuracy of the conversion from Greg Grochola's Au files in the x,y table format to the setfl format (Au-Grochola-JCP05.eam.alloy, conversion 15 December 2010 by C.A. Becker). The conversion was done by interpolating the table 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. 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: G. Grochola, S.P. Russo, and I.K. Snook, "On fitting a gold embedded atom method potential using the force matching method," J. Chem. Phys. 123, 204719 (2005).

The following input parameters were used with LAMMPS (4Aug10 version) for the fcc minimizations:

```
units      metal
boundary   p p p

atom_style atomic
lattice    fcc 4.070
region     box block 0 1.0 0 1.0 0 1.0
create_box 1 box
create_atoms 1 box

pair_style eam/alloy
pair_coeff  * * Au-Grochola-JCP05.eam.alloy Au

neighbor    1.0 bin
neigh_modify delay 0

minimize    0.0 1.0e-12 1000 100000
```

Comparison of minimum energies from LAMMPS and table 2 from the 2005 JCP reference:

Structure	a(A)	E_min(LAMMPS, eV/atom)	Value from Table 2 (eV/atom)	Notes
fcc	4.0701	-3.924217905475	-3.924	
E(bcc)-E(fcc)	3.222 (bcc)	0.06076892577	0.0608	
E(hcp)-E(fcc)	2.8780 (hcp)	0.009541435325	0.0095	c/a=1.630

To calculate the equilibrium volume at 1750 K, 4000 atoms corresponding to a liquid configuration were equilibrated for 1e6 steps using:

#3d simulation of EAM Au for Au-Grochola-JCP05.eam.alloy

```
units      metal
boundary   p p p
atom_style atomic
read_restart r.liquid_Al_1700
pair_style eam/alloy
pair_coeff  * * Au-Grochola-JCP05.eam.alloy Au
neighbor    1.0 bin
neigh_modify delay 0
thermo_style custom step temp press pe ke etotal vol lx ly lz pxx ppy pzz pxy pxz pyz
fix        1 all npt temp 1750.0 1750.0 1.0 iso 0.0 0.0 1.0
```

```
thermo      1000
timestep    0.001 # ps
restart     1000000 r
run         1000000
```

Then the following (NPT ensemble) was used for a “production” run to calculate the average volume for an average pressure of zero bars.

```
#3d simulation of EAM Au for Au-Grochola-JCP05.eam.alloy
units       metal
boundary    p p p
atom_style  atomic
read_restart r.1000000
pair_style  eam/alloy
pair_coeff   * * Au-Grochola-JCP05.eam.alloy Au
neighbor    1.0 bin
neigh_modify delay 0
thermo_style custom step temp press pe ke etotal vol lx ly lz pxx pyy pzz pxy pxz pyz
fix         1 all npt temp 1750.0 1750.0 1.0 iso 0.0 0.0 1.0
dump        1 all xyz 100000 dump.*
thermo      1000
timestep    0.001 # ps
restart     1000000 r
run         1000000
```

The result was an average volume of 76756 Angstroms³ with a standard deviation of 154. This gave a “unit cell” length of 4.2498 Angstroms. The average pressure was 31.107 bars with a standard deviation of 1783.7, corresponding to zero pressure. Considering just the simulation cell length (rather than volume), we get an average of 42.4984 Angstroms with a standard deviation of 0.0285. According to Dr. Grochola, they calculated a lattice constant of 4.249939195 Angstroms. Our results are consistent with those in Figure 3 of the article.





