

Day 2. Perfect Crystal in Pure Shear – Numerical Demonstrations

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1. Download and Compile MD++

Direct your browser to <http://micro.stanford.edu/~caiwei/Forum/2004-12-12-MD++/>
Download the latest MD++ source file, e.g. md++-2011-03-11.tar.gz, to your home directory.
You can also download the package using the `wget` command.

On your Unix/Linux workstation, do

```
$ cd ~  
$ wget http://micro.stanford.edu/~caiwei/Forum/2004-12-12-MD++/md++-2011-03-11.tar.gz  
$ mkdir Codes  
$ cd Codes  
$ tar zxvf ~/md++-2011-03-11.tar.gz
```

MD++ will be unzipped in the `~/Codes/MD++` directory.

To compile the code, do

```
$ cd MD++  
$ make eam build=R
```

This will create the executable `eam_gpp` in the `~/Codes/MD++/bin` directory. If you have intel compiler, you can use

```
$ make eam build=R SYS=intel
```

This will create the executable `eam_intel`, which may run faster than `eam_gpp`.

This executable implements the embedded-atom method (EAM) potential model, which works well for face-centered-cubic (FCC) metals, such as Cu.

More information about how to use MD++ can be found at:

[http://micro.stanford.edu/wiki/MD%2B%2B Manuals](http://micro.stanford.edu/wiki/MD%2B%2B+Manuals)

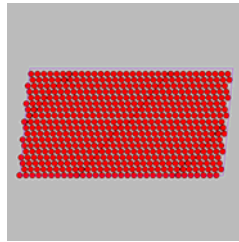
2. Shear Stress-Strain Relation at Zero Temperature

2.1. Run molecular static (MS) simulation

Execute the following commands.

```
$ cd ~/Codes/MD++  
$ bin/eam_gpp scripts/LLNL2010/Day2_create_0K_pure_shear_stress_cell.tcl \  
0.092
```

The argument (0.092) specifies γ_{xy} , the shear strain. The other strain components are adjusted iteratively during the simulation to make σ_{xy} the only non-zero stress component. The relaxed configuration is saved in directory: `runs/shear_copper/0K_092eps_112` . The simulation opens a window to display the following image showing the simulation cell.

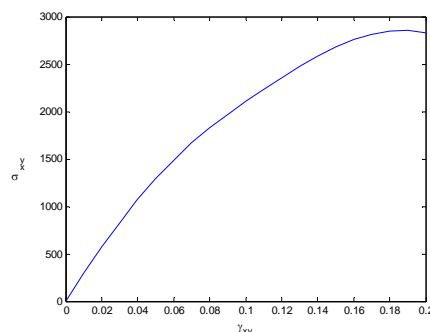


Use the following command to generate a shear stress-strain curve at zero temperature under the condition that σ_{xy} is the only non-zero stress component.

```
$ bin/eam_gpp scripts/LLNL2010/Day2_generate_0K_shear_stress_strain_curve.tcl
```

2.2. Process MS simulation results

The simulation data are stored in `stress.dat` and `strain.dat` the directory: `runs/shear_copper/0K_stressstrain` . These two files contain all the stress/strain components at the end of each relaxation. The ordering of the components is in `stress_info.dat` and `strain_info.dat` . The pure shear stress-strain curve at 0K is plotted below.



3. Shear Stress-Strain Relation at 300 K

The syntax for the molecular dynamics (MD) simulation command is the following.

```
$ bin/eam_gpp \  
  scripts/LLNL2010/Day2_create_non0K_pure_shear_stress_cell.tcl T strain
```

where

T : temperature (in K)
strain : engineering strain γ_{xy}

This will perform a series of MD simulations. At the end of each MD simulation, the simulation cell sizes is adjusted according to the average Virial stress with the goal to relax all the stress components other than σ_{xy} to zero.

As an example, execute the following commands.

```
$ cd ~/Codes/MD++  
$ bin/eam_gpp \  
  scripts/LLNL2010/Day2_create_non0K_pure_shear_stress_cell.tcl \  
  300 0.092
```

The data will be saved in the in `runs/shear_copper/300K_092eps_112strain` directory.

References:

[1] S. Ryu and W. Cai, "Entropic Effect on the Rate of Dislocation Nucleation",
<http://arxiv.org/abs/1011.1597>.

[2] S. Aubry, S. Ryu, K. Kang and W. Cai, "Energy Barrier for Homogeneous Dislocation Nucleation: Comparing Atomistic and Continuum Models", *Scripta Materialia*, in press, (2011).

Appendix A. Numerical Homework

1. Run MD simulations of EAM Cu (Mishin potential) in MD++ to find out the thermal strain at $T = 100, 200, 300, 600$ K. Plot the thermal strain as a function of temperature and estimate the thermal expansion coefficient.

2. Obtain the shear stress-strain relationship for the above potential model when σ_{xy} is the only non-zero stress component at $T = 0, 300, 600$ K, for x: [1 1 -2], y: [1 1 1], z: [1 -1 0].