Manual 02 for MD++

MD++ Tour with Sample Scripts

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1 Making a Perfect Crystal

Most solid materials have periodic crystal structure.[1] For example, copper and aluminum have the face centered cubic (FCC) structure, and molybdenum and tungsten do the body centered cubic (BCC) structure. The periodic array of atoms in solid gives benefits to the atomistic simulation. Mostly, we can use the periodic arrangement of atoms as the initial condition. Thus building the crystal structure can be regarded as the first step to the MD simulation of solids.In this section, we will learn how to build several common structures with sample script files in MD++.

1.1 Face centered cubic crystal

First of all, let's make a perfect crystal of aluminum, one of FCC crystals. You save the shell script in the bottom as 'al.script'[2] in the script directory. Then run the commands by typing

```
$ cd ~/Codes/MD++
$ bin/md_gpp scripts/al.script
```

The execution file, "md_gpp" is not eqipped with the potential model of the aluminum.[3] It will just show what the configuration will look like.

```
# -*-shell-script-*-
setnolog
setoverwrite
dirname = runs/al-example # specify run directory
```

[1] Glass is one of counter-examples, which is noncrystalline. We call it as amorphous material. In a sense that glass can flow (even at very slow rate), it can be sometimes considered as supercooled liquid rather than true solid.

[2] Basically, all the scripts explained here are already included in the directory "scripts/ME346", but I encourage you try to make a script.

[3] For the aluminum potential, you have to run "alglue_gpp".

```
#-------------------------------------------
# Create Perfect Lattice Configuration
#
crystalstructure = face-centered-cubic
latticeconst = 4.05 #(A) for Al
latticesize = [ 1  0  0  1  # c1 = 1*[1 0 0]
                0  1  0  1  # c2 = 1*[0 1 0]
                0  0  1  1] # c3 = 1*[0 0 1]
makecrystal
#-------------------------------------------------------------
# Plot Configuration
atomradius = 1.0 bondradius = 0.3 bondlength = 0
atomcolor = blue highlightcolor = purple backgroundcolor = gray
bondcolor = red fixatomcolor = yellow
plotfreq = 10 win_width = 600 win_height = 600
rotateangles = [ 0 0 0 1.0 ]
openwin alloccolors rotate saverot eval plot
sleep quit
```

The FCC crystal is one of close packed crystals together with HCP (Hexagonal Close Packed) crystal. For FCC crystal, you can imagine 8 corner atoms and 6 face-centered atoms in the cube. Since one corner atom is shared by 8 cubes and one face-centered atom is shared by 2 cubes, the total number of atoms per unit cell will be $8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4$ and their positions are shown in the Fig. 1(a), which you will get after you run the above command. The simulation cell can be extended by repeating the unit cell. If you change "latticesize" like

```
latticesize = [ 1  0  0  3
                0  1  0  3
                0  0  1  3]
```

you will see the three times bigger structure along the all x, y, and z directions in the Fig.1(b).

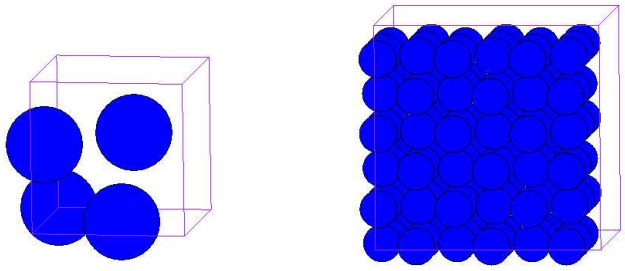
Ex.1 Make a perfect crystal of copper(Cu) of the latticesize [4],

$$\text{latticesize} = [\quad 1\,0\,0\,4$$
$$0\,1\,0\,4$$
$$0\,0\,1\,4]$$

Cu has FCC crystal structure and the lattice constant is 3.6030 Å. You can use either "md_gpp" or "eam_gpp". In case of "eam_gpp", you need to paste the following two lines into your script file after the line 'dirname'.

```
potfile = ~/private/MD/Codes/MD++/potentials/EAMDATA/eamdata.Cu
eamgrid = 5000 readeam
```

[4] In case of Cu or Al, the numbers of the fourth column in the variable, 'latticesize' shoul not be smaller than 4 due to their relatively long cut-off radius in this unit cell of [100],[010],and [001]. In the class, you will learn the criterion on the cell size, related with the cut-off radius.



(a) Unit Cell (b) 3X3X3 Cell

Figure 1: A perfect FCC aluminium crystal. (a) unit cell, $\mathbf{c}_1 = [100]$, $\mathbf{c}_2 = [010]$, and $\mathbf{c}_3 = [001]$ (b) 3×3×3 cell, $\mathbf{c}_1 = 3[100]$, $\mathbf{c}_2 = 3[010]$, and $\mathbf{c}_3 = 3[001]$ where $\mathbf{c}_i$'s are the periodicity vectors.

1.2 Body centered cubic crystal

For BCC crystal, which has 8 corner atoms and 1 body-centered atom in the unit cube, molybdenum is a good candidate for the demonstration. This time, we will use the Mo. potential model, "fs_gpp" instead of "md_gpp". You save the following script as 'mo.script' in the script directory. Then run MD++ by typing

```
$ bin/fs_gpp scripts/mo.script
```

```
# -*-shell-script-*-
setnolog
setoverwrite
dirname = runs/mo-example
#--------------------------------------------
# Read the potential file
potfile = ~/Codes/MD++/potentials/mo_pot readpot
#--------------------------------------------
# Create Perfect Lattice Configuration
crystalstructure = body-centered-cubic
latticeconst = 3.1472         # in Angstrom for Mo
latticesize = [  1  0  0  5
                 0  1  0  5
                 0  0  1  5 ]
makecrystal finalcnfile = perf.cn writecn
#--------------------------------------------
# Plot Configuration
atomradius = 1.0  bondradius = 0.3  bondlength = 0
```

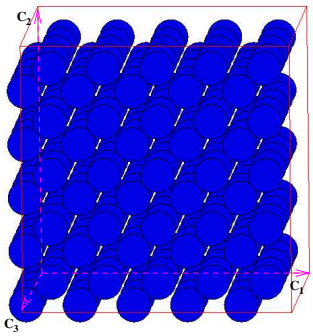


Figure 2: A perfect BCC molybdenum crystal. $\mathbf{c}_1 = 5[100]$, $\mathbf{c}_2 = 5[010]$, and $\mathbf{c}_3 = 5[001]$ are the periodicity vectors.

```
atomcolor = blue  highlightcolor = purple backgroundcolor = gray
bondcolor = red   fixatomcolor = yellow
plotfreq = 10  win_width = 600   win_height = 600
rotateangles = [ 0 0 0 1 ]
openwin alloccolors rotate saverot eval plot
sleep quit
```

In the Fig.2, the simulation box is defined by three periodicity vectors, $\mathbf{c}_1$, $\mathbf{c}_2$, $\mathbf{c}_3$:

$$\mathbf{c}_1 = 5[100], \mathbf{c}_2 = 5[010], \mathbf{c}_3 = 5[001].$$

The command *makecrystal* generates the perfect crystal of molybdenum based on the variables, *crystalstructure*[5] , *latticeconst*, and *latticesize*. The configuration is saved as "perf.cn" in the directory, runs/mo-example by the command *writecn*. The configuration file has the information of number of atoms and the position of all the atoms in terms of reduced coordiante followed by a 3×3 matrix, $\mathbf{H}$, whose columns are the three periodicity vectors, $\mathbf{c}_1$, $\mathbf{c}_2$, and $\mathbf{c}_3$. If you want to know the real coordinates of the atoms, you simply multiply the reduced coordinates by $\mathbf{H}$ like

$$\mathbf{r} = \mathbf{H} \cdot \mathbf{s}$$

where $\mathbf{r}$ is a vector of the real coordinate and $\mathbf{s}$ is a vector of the reduced coordinate.

Ex.2 Make a perfect crystal of tantalum(Ta). Ta has BCC lattice strucure and the lattice constant is 3.3058 Å. Read the following potential file for Ta.

```
potfile = ~/Codes/MD++/potentials/ta_pot readpot
```

[5]Other possible values for *crystalstructure* are "simple-cubic", "face-centered-cubic", "L1_2", "L1_0", "diamond-cubic", "zinc-blende", "hexagonal-ortho", "ice-Ih-0", and "ice-Ih".

1.3 Diamond cubic crystal

Basically, a diamond cubic crystal has two FCC crystals alternating by the offset vector, [111]/4 and the example materials are silicon and germanium. Just like our previous practice, run the following script, "si.script" by typing

```
$ bin/swsige_gpp scripts/si.script
```

, and you will see the graphical result like the Fig.3(b).

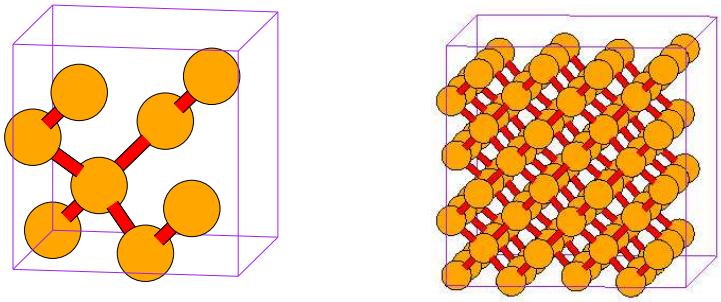
```
# -*-shell-script-*-
setnolog
setoverwrite
dirname = runs/si-example

#-------------------------------------------------------------
#Create Perfect Lattice Configuration
#
crystalstructure = diamond-cubic
latticeconst = 5.4309529817532409 #(A) for Si
latticesize = [ 1 0 0 2
                0 1 0 2
                0 0 1 2 ]
makecrystal  writecn
#-------------------------------------------------------------
#Plot Configuration
#
atomradius = 0.67 bondradius = 0.3 bondlength = 2.8285 #for Si
atomcolor = orange highlightcolor = purple
bondcolor = red backgroundcolor = gray70
plotfreq = 10  rotateangles = [ 0 0 0 1.25 ]
openwin alloccolors rotate saverot eval plot
sleep quit
```

1.4 Crystal structure of argon at low temperature

Argon is inert gas at room temperature but its solid state has face centered cubic crystal at low temperature(M.P.=83.81K). Using Leonard-Jones potential model, we can simulate the structure of solid argon.

```
$ bin/lj_gpp scripts/ar.script
```

```
# -*-shell-script-*-
setnolog
setoverwrite
```



(a) Unit Cell (b) 2×2×2 Cell

Figure 3: A perfect silicon crystal. (a) $\mathbf{c}_1 = [100]$, $\mathbf{c}_2 = [010]$, and $\mathbf{c}_3 = [001]$. (b) $\mathbf{c}_1 = 2[100]$, $\mathbf{c}_2 = 2[010]$, and $\mathbf{c}_3 = 2[001]$.

```
dirname = runs/ar-example # specify run directory

#-------------------------------------------
#Create Perfect Lattice Configuration
#
crystalstructure = face-centered-cubic
latticeconst = 5.260 #(A) for Ar
latticesize = [ 1  0  0  2
                0  1  0  2
                0  0  1  2]
makecrystal
#-----------------------------------------------------------------
#Plot Configuration
atomradius = 1.0 bondradius = 0.3 bondlength = 0
atomcolor = blue highlightcolor = purple backgroundcolor = gray
bondcolor = red fixatomcolor = yellow
plotfreq = 10 win_width = 600 win_height = 600
rotateangles = [ 0 0 0 1.0 ]
openwin alloccolors rotate saverot eval plot
sleep quit
```