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 face centered cubic (FCC) structures, while molybdenum and tungsten have the body centered cubic (BCC) structures. The periodic array of atoms in solid gives benefits to the atomistic simulation. Often, 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 FCC aluminum crystal. You can 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" does not give you any physical data as mentioned in the manual 01. It will just show what the configuration will look like.[3]

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

[1] Glass is one counter-example, which is noncrystalline, and we call it an amorphous material. It can be sometimes considered as supercooled liquid rather than true solid, in the sense that glass can flow at very slow rate.

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

[3] If you want aluminum potential to run, you have to execute "alglue_gpp" instead. You can compile it by typing `make alglue build=R`.

```
#-----------------------------------------
# Create Perfect Lattice Configuration
#
crystalstructure = face-centered-cubic
latticeconst = 4.05  # lattice constant for Al (unit: Angstrom)
latticesize = [ 1 0 0 1  # c1 = 1*[1 0 0] periodicity vec. in x
                0 1 0 1  # c2 = 1*[0 1 0] periodicity vec. in y
                0 0 1 1] # c3 = 1*[0 0 1] periodicity vec. in z
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, together with HCP (Hexagonal Close Packed) crystal, one of close packed crystals . For an FCC crystal, you can imagine 8 corner atoms and 6 face-centered atoms in the cube.(See Fig.1(a).) 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(b), 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

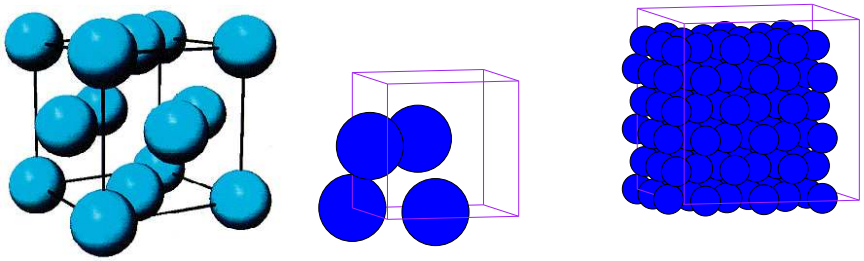
```
latticesize = [ 1  0  0  3
                0  1  0  3
                0  0  1  3]
```

you will see the three times bigger structure along the all x, y, and z directions in the Fig.1(b) and the variable *latticesize* defines the size of the simulation cell. The plot configuration part in the above script will be explained later in the manual 06.

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

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

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



(a) conventional view (b) unit cell (c) 3X3X3 cell

Figure 1: (a) A perfect FCC crystal has 8 cube corners and 6 face centers in one unit cell. (b) 4 atoms per unit cell, $\mathbf{c}_1 = [100]$, $\mathbf{c}_2 = [010]$, and $\mathbf{c}_3 = [001]$ (c) 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.

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

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

1.2 Body centered cubic crystal

For a BCC crystal, which has 8 corner atoms and 1 body-centered atom in the unit cell as shown in Fig.2(a), molybdenum(Mo) is a good candidate for the demonstration. This time, we use the Mo potential model, "fs_gpp" instead of "md_gpp". You can 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  3
                 0  1  0  3
                 0  0  1  3 ]
makecrystal finalcnfile = perf.cn writecn
#-------------------------------------------
# Plot Configuration
atomradius = 1.0  bondradius = 0.3  bondlength = 0
atomcolor = orange  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, $\mathbf{c}_1$, $\mathbf{c}_2$, $\mathbf{c}_3$:

$$\mathbf{c}_1 = 3[100], \mathbf{c}_2 = 3[010], \mathbf{c}_3 = 3[001].$$

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.

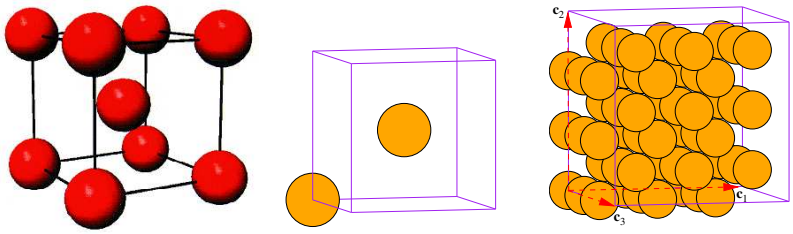
Ex.2 Make a perfect crystal of tantalum(Ta) with *latticesize*,

$$\text{latticesize} = \begin{bmatrix} 1 & 1 & 0 & 3 \\ 1 & -1 & 0 & 3 \\ 0 & 0 & 1 & 4 \end{bmatrix}.$$

Ta has a 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".



(a) conventional view (b) unit cell (c) 3×3×3 cell

Figure 2: (a) A perfect BCC crystal has 8 cube corners and 1 body centers in one unit cell. (b) 2 atoms per unit cell, $\mathbf{c}_1 = [100]$, $\mathbf{c}_2 = [010]$, and $\mathbf{c}_3 = [001]$ (c) 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.

1.3 Diamond cubic crystal

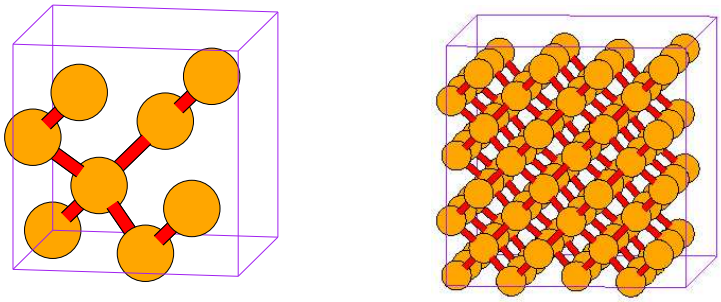
The diamond cubic crystal is two FCC crystals alternating by the offset vector, [111]/4 and the example materials are silicon and germanium. Just like our previous practice, run the following script, "si.script" by typing

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

, where the executable `sw_gpp` is the potential for Si, 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
#
```



(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 $\mathbf{c}_3 = 2[001]$.

```
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 a face centered cubic crystal at low temperature(M.P.=83.81K). Using the Leonard-Jones potential model, we can simulate the structure of solid argon.

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

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