Manual 02 for MD++

MD++ Tour with Sample Scripts

Keonwook Kang and Wei Cai

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1 Making a Perfect Crystal

Many solid materials have a periodic crystal structure.[1] For example, copper and aluminum have the face-centered-cubic (FCC) structure, while molybdenum and tungsten have the body-centered-cubic (BCC) structure under ambient conditions. The periodic arragement of atoms simplifies the process of setting up an atomistic simulation, because we can use a periodic array of atoms as the initial condition. Thus, building up a crystal structure is often the first step in an MD simulation of solids. In this manual, we will learn how to build several crystal structures in MD++ through a few examples.

1.1 Face-centered-cubic crystal

First, let's make a perfect FCC aluminum crystal. The script file `al.script`, together with other script files discussed in this manual, can be found in the directory `MD++/scripts/ME346`. To run this script file, type

```
$ cd ~/Codes/MD++
$ bin/md_gpp scripts/ME346/al.script
```

The executable file, `md_gpp` does not contain any potential model, but can be used for visualization purposes, as mentioned in the Manual 01.[2] Here is the content of the `al.script` file.

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

[1] Glass is a counter-example, which is noncrystalline. We call it an amorphous material. Sometimes people consider it as supercooled liquid instead of a true solid, because, like a liquid, glass can flow under shear stress, although at very slow rate.

[2] You can obtain the executable `alglue_gpp`, which contains a "glue" potential model for aluminum by `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
```

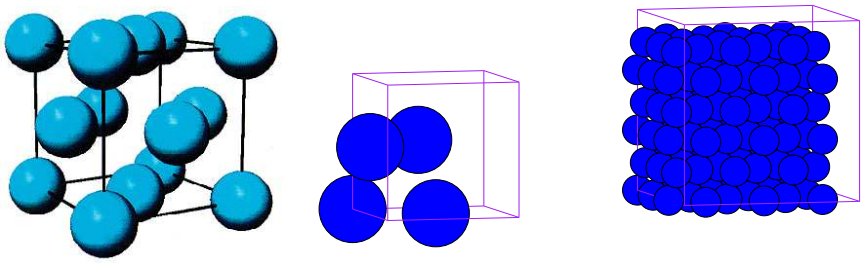
FCC, as well as HCP (Hexagonal Close Packed), is a close-packed crystal structure. To visualize the FCC structure, you may consider a cube shown in Fig. 1(a), where there is an atom in every corner and every face center of the cube. The cube is called a unit cell. Now imagine that the unit cell is replicated periodically in all 3 directions to fill the entire space. This forms an infinitely large crystal. Since each corner atom is shared by 8 adjacent cubes and each face-centered atom is shared by 2 cubes, the total number of atoms per unit cell will be $8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4$. If we associate each atom with only one unit cell, then these four atoms can be plotted as in Fig.1(b), which is what you will observe if you run `al.script`. We can create a larger crystal (containing more than 1 unit cell) by modifying the `latticesize` variable, e.g.

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

This creates a crystal with $3 \times 3 \times 3 = 27$ unit cells as shown in the Fig.1(c). The `plot` section of this script file will be explained in Manual 06.

Exercise 1 Make a perfect crystal of copper (Cu) containing $4 \times 4 \times 4$ unit cells. [3], Cu has an FCC crystal structure and its equilibrium lattice constant is a =3.6030 Å. You can use `md_gpp` as the executable file if you only want to

[3]For MD simulations of Cu or Al, the fourth column of `latticesize` should not be smaller than 4 due to the relatively large cut-off radius in their potential models (`eam` or `alglue`).



(a) conventional view (b) unit cell (c) $3 \times 3 \times 3$ 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 of the simulation supercell.

visualize the structure. Use `eam_gpp` if you would also want to do some computation using the potential model. (For example, the `eval` command computes the total potential energy of the structure.) For the latter case, 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
```

This reads in the data needed by the EAM potential model of Cu.

Exercise 2 Make a perfect crystal of argon (Ar) containing $4 \times 4 \times 4$ unit cells. Argon is inert gas at room temperature but its solid state has a face centered cubic crystal below its melting temperature $T_m = 83.81$K. Ar can be described by the Leonard-Jones potential model, which is contained in the executable `lj_gpp`. Modify `scripts/ME346/ar.script` and run it with

```
$ bin/lj_gpp scripts/ME346/ar.script
```

1.2 Body-centered-cubic crystal

The BCC structure has an atom at every corner and body-center of each cube (unit cell), as shown in Fig.2(a). Here we use molybdenum (Mo) as an example. Run "mo.script" file by typing

```
$ bin/fs_gpp scripts/ME346/mo.script
```

Here is the content of the `mo.script` file.

```
# -*-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(c), the simulation box (i.e. supercell) is defined by three periodicity vectors, $\mathbf{c}_1$, $\mathbf{c}_2$, $\mathbf{c}_3$:

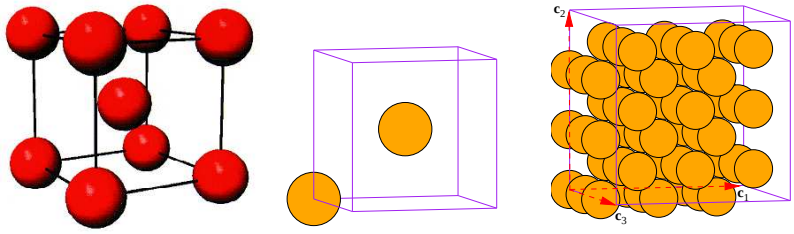
$$\mathbf{c}_1 = 3[100], \mathbf{c}_2 = 3[010], \mathbf{c}_3 = 3[001].$$

The command `makecrystal` generates the perfect crystal of molybdenum based on the variables, `crystalstructure`[4] , `latticeconst`, and `latticesize`. The configuration is saved as "perf.cn" in the directory 'runs/mo-example' by the command `writecn`. The configuration file contains the number of atoms and the position of all the atoms in terms of scaled coordinates followed by a 3×3 matrix, $\mathbf{H}$, whose columns are the three periodicity vectors, $\mathbf{c}_1$, $\mathbf{c}_2$, and $\mathbf{c}_3$. The real coordinates of an atom, $\mathbf{r} = (x, y, z)^T$ is related to the scaled coordinates $\mathbf{s} = (s_x, s_y, s_z)^T$ through matrix multiplication

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

Exercise 3 Make a perfect crystal of tantalum (Ta) with repeat vector $\mathbf{c}_1 = 3[1\,1\,0]$, $\mathbf{c}_2 = 3[1\,\bar{1}\,0]$, $\mathbf{c}_3 = 4[0\,0\,1]$. Ta has a BCC lattice structure with an equilibrium lattice constant $a_0 = 3.3058\mathring{A}$. Read the FS potential file for Ta by `potfile = ~/Codes/MD++/potentials/ta_pot readpot`

[4]Other possible values for `crystalstructure` are "simple-cubic", "face-centered-cubic", "L1_2", "L1_0", "diamond-cubic", "zinc-blende", etc. For a complete list, please read `src/lattice.h`.



(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

Si has the diamond cubic structure, which can be regarded as two FCC structures offset by [1 1 1]/4. You can run the script `si.script` by typing

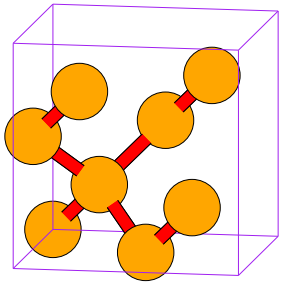
```
$ bin/sw_gpp scripts/ME346/si.script
```

where the executable `sw_gpp` contains the SW potential model for Si. The visualization window will look like Fig.3(b).

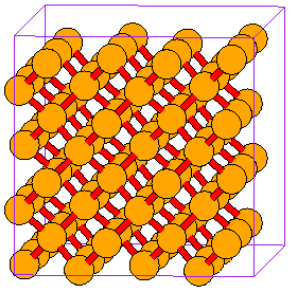
Here is the content of the `si.script` file.

```
# -*-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
```



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

```
atomcolor = orange highlightcolor = purple
bondcolor = red backgroundcolor = gray70
plotfreq = 10  rotateangles = [ 0 0 0 1.25 ]
openwin alloccolors rotate saverot eval plot
sleep quit
```