Manual 03 for MD++

MD++ Tour with Sample Scripts

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1 Reading a Log File

In the previous example scripts, the command, *setnolog* was activated and a lot of the information related with the simulation was printed out to standard output , which is usually your terminal screen. If you want to keep the record of this information, you can comment out *setnolog*, which will generate a log file *A.log* in your running directory. For example, if you run "mo.script" in the previous manual with *setnolog* commented out, then you will find the A.log file in the "runs/mo-example" directory. To read this file, type

```
$ more runs/mo-example/A.log
```

Basically, you see the same content as you previously saw on the terminal. In the log file, the lines starting with "ASSIGN" show the declaration of certain variables and the lines with "EXEC" correspond to the execution of the commands. Some important properties such as number of atoms(_NP), potential energy (EPOT), kinetic energy (KATOM), pressure (PRESSURE), stress (Stress) are also listed in the file, if you have the command *eval* in the script. At the end of the simulation, the log file may be zipped into "A.log.gz", in which case you can use

```
$ gzip -cd runs/mo-example/A.log.gz | more
```

to see the content. If you want to find certain data (e.g. EPOT) in the log file, you may use

```
$ grep EPOT runs/mo-example/A.log
```

or

```
$ gzip -cd runs/mo-example/A.log.gz | grep EPOT
```

In case that you want to "grep" several lines following your keyword (e.g. Stress), you can use

```
$ grep -3 Stress runs/mo-example/A.log
```

which shows three lines above and below the line containing the keyword "Stress".

2 Lattice Energy and Bulk Modulus

Silicon has the diamond cubic (DC) crystal structure. In this section, we will compare DC structure of silicon with other hypothetical crystal structures such as face-centered-cubic(FCC), body-centered-cubic(BCC), and simple-cubic(SC) in terms of the energy per atom at 0K. We will see that the DC structure has the lowest energy, hence, it is the most favored crystal strucure for silicon. The lattice energy, Φ and the number density, ρ are defined by

$$\begin{aligned} \Phi &= \frac{E_{pot}}{N} \\ \rho &= \frac{N}{V} \end{aligned}$$

where E_{pot} is the potential energy of the system, N is number of atoms in the simulation cell and V is the volume of the simulation cell. Now, run the following script using SW potential model.

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

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

#-------------------------------------------------------------
#Create Perfect Lattice Configuration
#
crystalstructure = diamond-cubic
latticeconst = 5.4309529817532409 #(A) for Si
latticesize = [ 1 0 0 3
                0 1 0 3
                0 0 1 3 ]
makecrystal eval

latticeconst = 4.850 makecrystal eval
latticeconst = 4.950 makecrystal eval
latticeconst = 5.050 makecrystal eval
                :
(many lines omitted here for brevity)
                :
```

```
latticeconst = 5.900 makecrystal eval
latticeconst = 6.000 makecrystal eval
latticeconst = 6.100 makecrystal eval


crystalstructure = face-centered-cubic

latticeconst = 4.105 makecrystal eval
latticeconst = 4.110 makecrystal eval
                :
                :
latticeconst = 4.205 makecrystal eval
latticeconst = 4.215 makecrystal eval



crystalstructure = body-centered-cubic

latticeconst = 3.210 makecrystal eval
latticeconst = 3.220 makecrystal eval
                :
                :
latticeconst = 3.320 makecrystal eval
latticeconst = 3.340 makecrystal eval


crystalstructure = simple-cubic

latticeconst = 2.550 makecrystal eval
latticeconst = 2.600 makecrystal eval
                :
                :
latticeconst = 2.640 makecrystal eval
latticeconst = 2.650 makecrystal eval
quit
```

From the log file, you can find number of atoms for the $3 \times 3 \times 3$ DC cell to be 216. you can also obtain this number $8 \times 3^3 = 216$, since there are eight atoms in the DC unit cell. For other crystal strucures, the number of atoms in the $3 \times 3 \times 3$ cell is given in the following table.

Crystal Structure	No. of atoms in the unit cell	Total No. of atoms
SC	1	27
BCC	2	54
FCC	4	108
DC	8	216

The potential energy at each different lattice constant can also be read from the log file by typing

```
$ grep EPOT runs/si_polytype/A.log
```

The volume of a simulation cell can be obtained from the determinant of the matrix H.[1] When H is a triangular matrix,

$$V = \det(H) = H(1,1)H(2,2)H(3,3)$$

the volume is the product of the entries in the main diagonal. The unit of volume is $\mathring{A}^3$. From these, we can calculate the lattice energy, Φ of silicon for different number density ρ, and plot (ρ, Φ) for different crystal structures as shown in Fig.1(a)[1] and Fig.1(b)[2]

From the result, we can also calculate the bulk modulus of DC silicon. The bulk modulus is defined as [2]

$$B = V \frac{\partial^2 \Phi}{\partial V^2}_{V=V_0} \tag{1}$$

where V_0 is the atomic volume of silicon at the energy minimum. For small deformations, the energy around the energy minimum is approximately a quadratic function of the atomic volume.(See Fig.1(b).) The coefficient of quadratic term in the 2nd order polynomial is obtained by the matlab command *polyfit* and it is 0.0169 eV/Å^6. Evaluating the equation 1 at the atomic volume of lowest energy state ($V_0 = 20.025$Å^6) gives

$$B = 2 \times 20.025\,\text{Å}^3 \times 0.0169\,\text{eV/Å}^6 \times 160\,\text{GPa/(eV/Å}^3) = 108.3\,\text{GPa}$$

This result is in exact accordance with that of Balamane *et al*'s paper.[3] From the elasticity theory, the bulk modulus, B is defined as

$$B = \lambda + \frac{2}{3}\mu \qquad \text{for isotropic material}$$

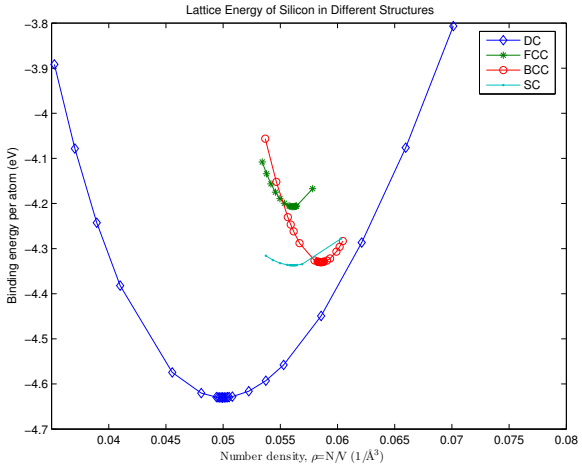
$$B = \frac{1}{3}(C_{11} + 2C_{12}) \qquad \text{for cubic material}$$

where λ and μ are Lame's constants and C_{11} and C_{12} are elastic constants. Since Si has $C_{11} = 165.7$ GPa and $C_{12} = 63.9$ GPa [4] , the bulk modulus, B is 98.4 GPa, which is a bit different from the atomistic calculation.[3] This difference is mainly dependent on what potential model is used for the simulation. In the reference [3], various potential models predict slightly different elastic constants.

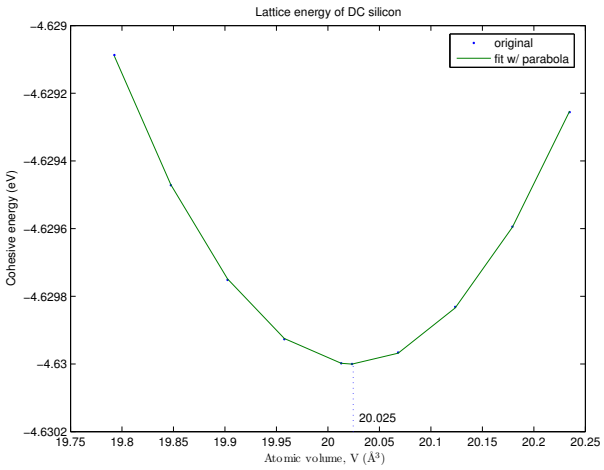
[1] The matrix H defines the size and shape of the simulation cell. $H = [\mathbf{c}_1\,\mathbf{c}_2\,\mathbf{c}_3]$ where $\mathbf{c}_i$'s are three periodicity vectors.

[2] $B = -V\partial P/\partial V$ and $P = -\partial\Phi/\partial V$.

[3] Lately, I found a paper, which says the bulk modulus of DC Si with Stillinger-Weber potential is 94 GPa, much closer to 98.4 GPa. [5]



(a) Si in different crystal structures



(b) Lattice energy of Si DC

Figure 1: (a) The lattice energy of silicon for four different crystal structures (DC, FCC, BCC, and SC) are plotted as number density. Silicon has the lowest binding energy when it forms diamond cubic structure. (b) The lattice energy of DC silicon as a function of the atomic volume is fitted with a parabola (dash-dot line) and with spline interpolation (solid line).

References

[1] F. H. Stillinger and T. A. Weber, PRB **31** 5262-5271

[2] J. Tersoff PRB **37** 6991-7000

[3] H. Balamane, T. Halicioglu, and W. A. Tiler, PRB **46** 2250-2279

[4] J. P. Hirth and J. Lothe, "*Theory of Dislocations*"

[5] R. L. C. Vink, G. T. Barkema, W. F. van der Weg, and N. Mousseau, "Fitting the Stillinger-Weber potential to amorphous silicon", J.Non-Cryst. Solids **282** 248 (2001).