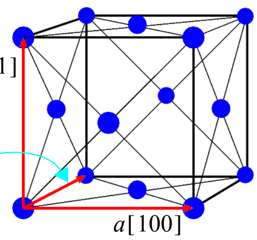
Molecular dynamics 2015

Exercises 1 to chapter 1: Visualization



The face-centered cubic (FCC) lattice structure is as follows: a lattice has an number of cubes next to each other. Each cube has an atom in each corner, and in addition there is an atom on the center of each side of the cube. One cube is called the unit cell, and it thus has 4 atoms in total (Why only 4?). By displacing the atoms a bit it is possible to make a cube which has four atoms inside it.

FCC is one of the two close-packed structures in 3D, the other one is hexagonal close packed (HCP). The statement that FCC and HCP are the tightest ways of packing spheres in 3D is called the Kepler conjecture. All physicists know it's true but mathematicians only recently have been able to prove it (http://mathworld.wolfram.com/KeplerConjecture.html).

1. **(12 p)** Write a program which creates a 3-dimensional Cu FCC-lattice and prints it out in the XYZ format. As input the program should read the size of the system in unit cells in each direction (x, y, z). Coordinates of the atoms in the XYZ file should be in Å. Make a figure out of a $4 \times 4 \times 4$ system and visualize this with `rasmol, ovito or dpc`[1] so that at least three sides of the cube are visible. The lattice constant of Cu (side length of unit cell) is $a = 3.62$ Å.

2. **(8 p)** Modify your program so that you can visualize the (111) surface of the Cu FCC lattice. You can do this either by cutting the cube in the right direction or building the system from unit cells with the right orientation (i.e. a unit cell with one side in the (111) plane; it is possible, we come to that later in the lectures). Check that you get the right symmetry in the (111) plane (hexagonal).

The exercises are returned by emailing the source code creating atoms and one `rasmol`-picture/exercise in the gif format.

For additional information about crystal structures and notation see any solid state physics textbook, e.g. Kittel or Ashcroft and Mermin. Shortly, plane (111) is the the plane that is perpendicular to the vector $[111] = \mathbf{i} + \mathbf{j} + \mathbf{k}$. Here the unit vectors are oriented along the edges of the cube depicted above.

1. Or whatever visualization program you use.