1 Exercise 1 - Atomic packing factor

a. Simple Cubic

Solution: Before all this we need to perform a quick calculation to know the radius of the atoms, assuming they are spherical and have a volume equal to V_atom,

$$V_{atom} = \frac{4}{3}\pi r^3,$$
$$\Rightarrow r_{atom} = \left(\frac{3V_{atom}}{4\pi}\right)^{1/3}. \tag{1}$$

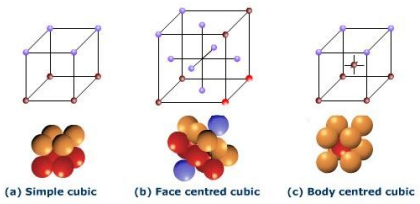

Figure 1: a) SC, b) FCC and c) BC unit cells (image taken from *http://chem-guide.blogspot.de/2010/04/simple-cubic-face-centered-and-body.html*).

Now that we know this we can start with the main calculations. First the atomic packing factor for the SC unit cell. For this cell we have atoms placed at the corners of a cube. They touch along the side of the cube as we can see in fig. 1. Hence the length of the size of the cube is

$$a = r + 2 = 2r,$$

So the volume of the unit cell is

$$V_{cell} = a^3 = 8r^3 = 8\frac{3V_{atom}}{4\pi} = \frac{6V_{atom}}{\pi}, \tag{2}$$

There is just 1 atom inside the unit cell, so the atomic packing factor is going to be

$$APF_{SC} = \frac{NV_{atom}}{V_{cell}} = \frac{(1)V_{atom}}{\frac{6V_{atom}}{\pi}} = \frac{\pi}{6}, \tag{3}$$

b. FCC

Solution: Now for the FCC we can see that now we have atoms at the corners and in the center of each face, so now the atoms are touching along the diagonal of the faces of the cube. So the diagonal size must be

$$c = r + 2r + r = 4r, \tag{4}$$

but we are not interested in the diagonal, we want to know the size of the sides. We can obtain such

sides with basic trigonometry, if a is the side length then

$$\begin{aligned} c^2 &= (4r)^2 = 16r^2, \\ c^2 &= a^2 + a^2 = 2a^2, \\ \Rightarrow 8r^2 &= a^2 \\ \Rightarrow a &= \sqrt{8}r. \end{aligned} \tag{5}$$

Therefore the volume of the unit cell is

$$V_{cell} = (\sqrt{8}r)^3 = 8\sqrt{8}r^3 = 16\sqrt{2}r^3 = 16\sqrt{2}\frac{3V_{atom}}{4\pi} = \frac{12\sqrt{2}V_{atom}}{\pi}. \tag{6}$$

The FCC cell has 4 atoms, $8 * (1/8) + 6 * (1/2)$, the $1/8$ comes from the atoms on the corner that are in 8 cells simultaneously and the $1/2$ comes from the atoms in the faces that are shared by two cells each. So the packing factor is

$$APF_{FCC} = \frac{4 * V_{atom}}{V_{cell}} = \frac{4 * V_{atom}}{\frac{12\sqrt{2}V_{atom}}{\pi}} = \frac{\pi}{3\sqrt{2}} \tag{7}$$

2 Exercise 2 - Bravais lattice

a. Why don't vector $\vec{a}$ and $\vec{b}$ form a Bravais lattice?

Solution: In this case such vectors don't form a Bravais Lattice because a Bravais lattice must look the same for every $\vec{R} = n_1\vec{a} + n_2\vec{b}$, with $n_1, n_2 \in \mathbb{Z}$, and this is not the case for this choice of primitive vectors. For example for the two points depicted in fig. 1 the lattice will not look the same

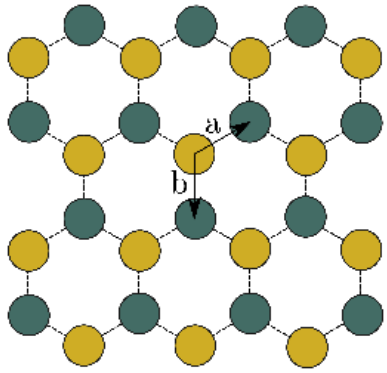

Figure 2: Example of two points for which the lattice is not going to look the same

b. How can one construct a Bravais lattice for this system?

Solution:

We can actually create a Bravais lattice if we change the primitive vectors and define the basis as shown in fig. 2

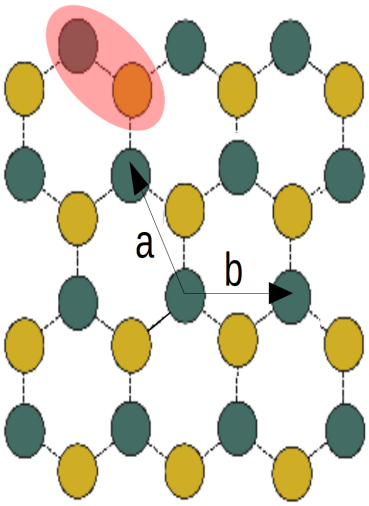

Figure 3: New primitive vectors and new basis to turn the honeycomb into a Bravais lattice. The new vectors are also named $\vec{a}, \vec{b}$ and the basis is enclosed on the ellipse on the top left part of the image.

c. Construct the Wigner-Seitz cell for this Bravais lattice.

Solution:

In fig. 3 we can see the construction of the Wigner-Seitz cell. Basically we draw lines between first neighbors. After that we draw the median to the lines drawn on the last step. And finally the cell we are looking for will be the volume comprised inside the medians drawn on the second step.

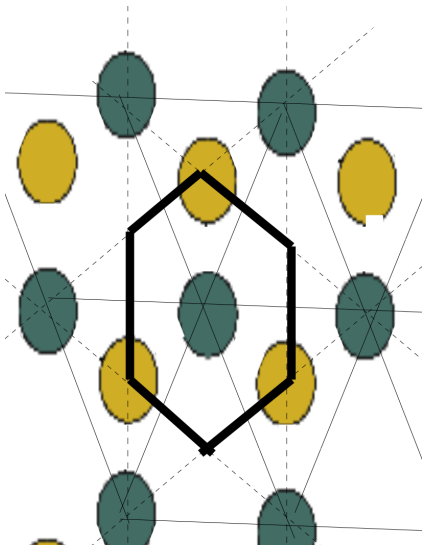

Figure 4: Wigner-Seitz cell for the our Bravais lattice. The solid thin lines are connections between first neighbors. The dashed lines are the medians to the lines joining first neighbors. The solid wide lines are then the limits of the Wigner-Seitz cell.

3 Exercise 3 - Crystal symmetries

4 Exercise 4 - Cairo tiling