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},

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

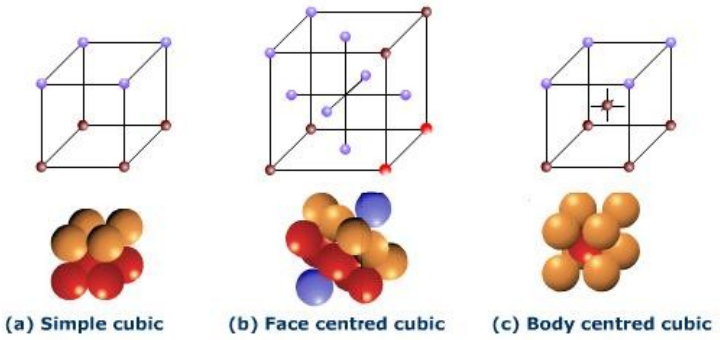

Figure 1: a) SC, b) FCC and c) BCC unit cells (image taken from *http://chem-guide.blogspot.de/2010/04/simple-cubic-face-centered-and-body.html*).

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

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

c. BCC

Solution: Now it is time to do the same calculations for the BCC unit cell. In such cell we have atoms on every corner of the cube and an extra one placed at the center. So now the atoms touch each other alongside the diagonal. As a result, the diagonals of the cell have a length of

$$c = r + 2r + r = 4r.$$

By basic trigonometry we know that the size of the diagonal of a cube is $c = \sqrt{3}a$, where a is the size of each side. So the length of the diagonal in terms of the atomic radius is

$$\begin{aligned} \sqrt{3}a &= 4r, \\ \Rightarrow a &= \frac{4}{\sqrt{3}}r = \frac{4}{\sqrt{3}}\left(\frac{3V_{atom}}{4\pi}\right)^{1/3}. \end{aligned} \tag{8}$$

As a consequence, the volume of the cell is

$$V_{cell} = a^3 = \frac{64}{3\sqrt{3}}\left(\frac{3V_{atom}}{4\pi}\right) = \frac{16V_{atom}}{\sqrt{3}\pi}. \tag{9}$$

The number of atoms in a BCC cell is 2, $(8 * 1/8 + 1)$, one in the center and 8 on the corners contributing $1/8$ each, knowing this the atomic packing factor is

$$APF_{BCC} = \frac{2 * V_{atom}}{V_{cell}} = \frac{2 * V_{atom}}{\frac{16V_{atom}}{\sqrt{3}\pi}} = \boxed{\frac{\sqrt{3}\pi}{8}}. \tag{10}$$

d. HCP

Solution: The only remaining structure to calculate here is the HCP unit cell. In fig. 2 we can see the scheme we will use to perform our calculations.

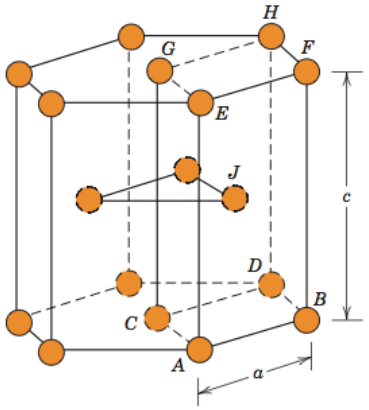

Figure 2: HPC structure, taken from *https://www.e-education.psu.edu/matse81/node/2134*.

Let's consider the tetrahedron formed by the vertexes $ABCJ$. It's is easy, with our now acquired experience, to see that atoms are touching each other alongside AB, and also along BJ, both these sides have the same length $a = 2r$. So far we are not in troubles, so let's calculate the height of the tetrahedron $c/2$. We know that the triangle ABC is equilateral, as ABJ, BCJ and CAJ, therefore we have a tetrahedron with equilateral triangles as faces, so J must lie right above the centroid of the triangle

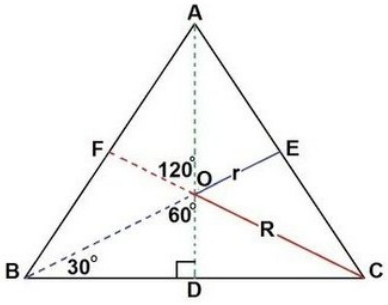

Figure 3: Centroid of an equilateral triangle, taken from *https://www.quora.com/What-is-the-centroid-of-equilateral-triangle*.

In fig. 3 we want to know the length of BO, we know that $BD = a/2$, if we use the definition of cosine then we will find

$$\cos(30°) = \frac{\sqrt{3}}{2} = \frac{BD}{BO},$$
$$\Rightarrow BO = \frac{2BD}{\sqrt{3}} = \frac{a}{\sqrt{3}} \tag{11}$$

Now using Pythagoras theorem we find OJ (remember that $OJ = c/2$)

$$BJ^2 = BO^2 + OJ^2,$$
$$a^2 = \frac{a^2}{3} + OJ^2,$$
$$OJ = \frac{\sqrt{2}a}{\sqrt{3}}, \tag{12}$$

then

$$c = 2OJ = \frac{2\sqrt{2}a}{\sqrt{3}}. \tag{13}$$

We almost finish, we just need to know the apothem size (CF), this can be easily calculated with Pythagoras theorem and eq. 11

$$CF^2 = a^2 - \frac{a^2}{4} = \frac{3a^2}{4},$$
$$\Rightarrow CF = \frac{\sqrt{3}a}{2}. \tag{14}$$

The area of the base hexagon is then

$$Area_{hex} = \frac{6a * CF}{2} = \frac{3\sqrt{3}a^2}{2}, \tag{15}$$

hence the volume of the unit cell is

$$\begin{aligned} V_{cell} = c * Area_{hex} &= \frac{2\sqrt{2}a}{\sqrt{3}}\frac{3\sqrt{3}a^2}{2} \\ &= 3\sqrt{2}a^3 = 3\sqrt{2}(2r)^3 = 24\sqrt{2}r^3 = \\ &= 24\sqrt{2}\frac{3V_{atom}}{4\pi} = \frac{18\sqrt{2}V_{atom}}{\pi}. \end{aligned} \tag{16}$$

And finally we can calculate the atomic packing factor. In the hcp cell there are 6 atoms ($6*1/4+3$), hence we have

$$APF_{HCP} = \frac{6 * V_{atom}}{V_{cell}} = \frac{6 * V_{atom}}{\frac{18\sqrt{2}V_{atom}}{\pi}} = \boxed{\frac{\pi}{3\sqrt{2}}}. \tag{17}$$

e. Crystal structure of iron

Solution: This one might be tricky. Let's first define the density in the unit cell.

$$\rho = \frac{NM_{atom}}{V}. \tag{18}$$

Assuming we have a cubic cell, we can use $V = a^3$. Hence, from the density, mass, and volume, we can know how many atoms are there inside the unit cell.

$$N = \frac{\rho V}{M_{atom}}. \tag{19}$$

If we plug the numbers in the computer (using the appropiate units), we will find that $N \approx 2.0022590256465516$, which is very close to 2. And two is the number of atoms inside a BCC cell. Therefore **the crystal structure of the iron is BCC.**

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. 4 the lattice will not look the same

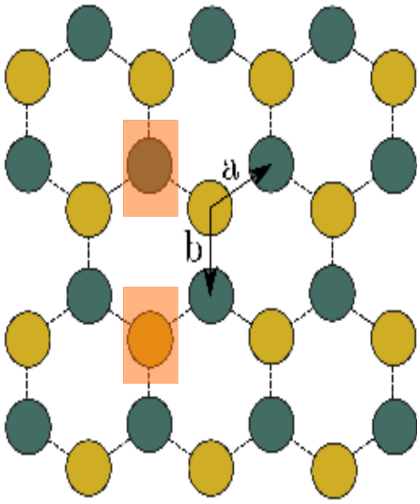

Figure 4: Example of two points for which the lattice is not going to look the same

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. 5

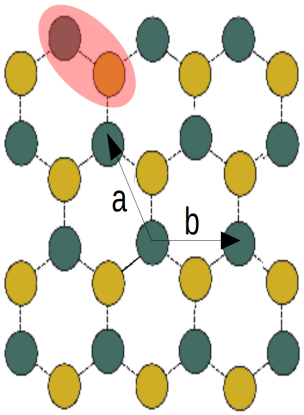

Figure 5: New primitive vectors and new basis to turn the honeycomb into a Bravais lattice. The new vectors are also named $\vec{a}, \vec{b}$ and the basis is enclosed on the ellipse on the top left part of the image.

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

Solution:

In fig. 6 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.

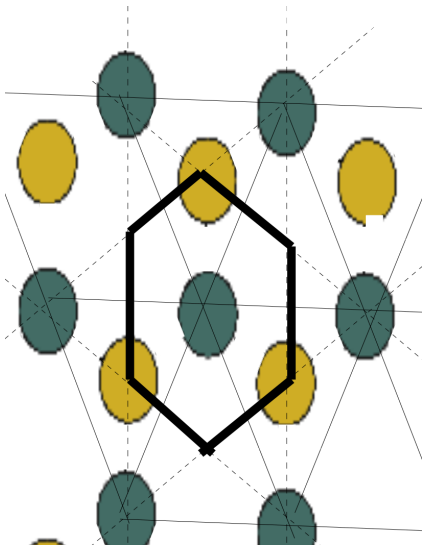

Figure 6: Wigner-Seitz cell for the our Bravais lattice. The solid thin lines are connections between first neighbors. The dashed lines are the medians to the lines joining first neighbors. The solid wide lines are then the limits of the Wigner-Seitz cell.

3 Exercise 3 - Crystal symmetries

a. No 5-fold symmetry

Solution: The short answer to why there is no 5-fold symmetries in crystals is, because we can not cover a plane (space) entirely using only regular pentagons.

We can also show an interesting proof using a shrinking argument. We know that a rotation symmetry must move a lattice point to a succession of other lattice points. In other words, a rotation must move lattice points to other lattice points. Now let's set up our rotations

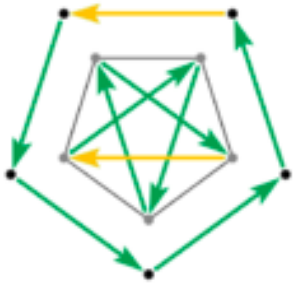

Figure 7: Translation vectors for a $2\pi/5$ rotation in a "pentagonal lattice". Taken from *http://enacademic.com/dic.nsf/enwiki/1056789*.

If a displacement exists between any two lattice points, then that displacement must repeat in every point of the lattice. Now let's take a point and construct a 5-point star joining the displacement vectors head to tail. As we know, all this points must be lattice points, but now the pentagon is smaller, and this cannot be possible, because this implies that the new "shrinked" points were also lattice points. We can repeat this process again and again until we can make the lattice points as close as we want, therefore modifying the lattice. If we had a rotation symmetry this wouldn't be possible, since the lattice under such rotations should be exactly the same. Therefore proving that a 5-fold symmetry is indeed impossible. ■

b. Quasicrystalls

Solution: Quasicrystals are physical lattices with translational disorder that retain local, rotational symmetry. This means that crystalls have rotational and translational symmetries, while quasycristalls only have rotational symmetry, so if we move the lattice, the translated lattice will not match the original one.

4 Exercise 4 - Cairo tiling

a. Bravais lattice of Cairo tiling

Solution: We can see the found Bravais lattice in fig. 8. We can spot it easily, by only joining the intersection points of the tiles making right angles.

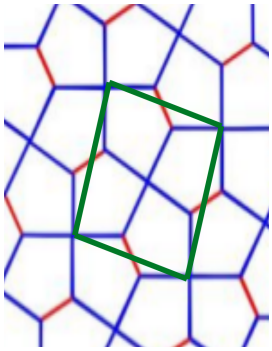

Figure 8: Cell of the Bravais lattice for Cairo tiling

b. Primitive cell vectors and angle between them

Solution: The desired elements are shown in fig. 9, the angle ϕ will be used on the next question.

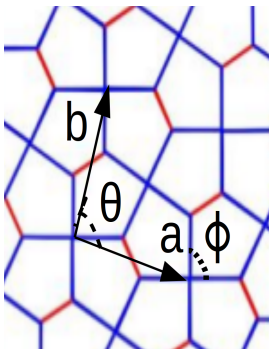

Figure 9: Primitive vectors and angle between them on the unit cell of Cairo Tilings

c. Determine the value of θ

Solution: It's easy to show, by using corresponding angles, that $\theta = \phi$, and since $\phi = \pi/2$ we have by transitivity that $\theta = \pi/2$

d. Tilings inside a unit cell

Solution: There are **4 tiles within a unit cell**.