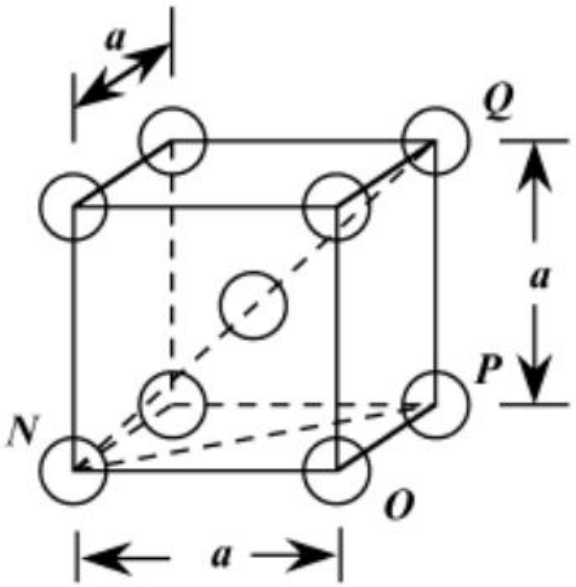
# Fundamentals of Materials Science
# Homework 7, SS 2017

Complete the following problems. You are expected to show the detailed steps and make necessary sketches or drawings on how you have arrived at the final results.

1. Please describe in your own understanding what the crystal structure is. You are expected to describe in both Chinese and English. Your description should be from two directions as I discussed in class. One is from Space Lattice to Crystal Structure, while the other way is to extract the concept of Space Lattice from Crystal Structure. Please show me that you really understand the concept.

2. Show for the body-centered cubic crystal structure that the unit cell edge length $a$ and the atomic radius $R$ are related through $a = 4R/\sqrt{3}$.

Consider the BCC unit cell shown below




Using the triangle $NOP$

$$(\overline{NP})^2 = a^2 + a^2 = 2a^2$$

And then for triangle $NPQ$,

$$(\overline{NQ})^2 = (\overline{QP})^2 + (\overline{NP})^2$$

But $\overline{NQ} = 4R$, $R$ being the atomic radius. Also, $\overline{QP} = a$. Therefore,

$$(4R)^2 = a^2 + 2a^2$$

or

$$a = \frac{4R}{\sqrt{3}}$$

3. Calculate the atomic radius in cm for the following: (a) BCC metal with a = 0.3294 nm; and (b) FCC metal with a = 4.0862 Å.

**Solution:**

For BCC metals:

$$r = \frac{\sqrt{3}}{4} a_0$$

$$r = \frac{\sqrt{3}}{4}(0.3294\ \text{nm}) = 0.1426\ \text{nm}$$

$$\boxed{r = 1.426 \times 10^{-8}\ \text{cm}}$$

For FCC metals:

$$r = \frac{\sqrt{2}}{4} a_0$$

$$r = \frac{\sqrt{2}}{4}(4.0862\ \text{Å}) = 1.4447\ \text{Å}$$

$$\boxed{r = 1.4447 \times 10^{-8}\ \text{cm}}$$

4. Calculate the lattice parameter of each of the following elements using their atomic radii: (a) iron, (b) aluminum, (c) copper, and (d) magnesium.

**Solution:**

Iron is BCC and the $a_0$ to $r$ relationship is

$$a_0 = \frac{4}{\sqrt{3}} r = \frac{4}{\sqrt{3}} (1.24)$$

$$\boxed{a_0 = 2.86 \text{ Å}}$$

Aluminum is FCC and the $a_0$ to $r$ relationship is

$$a_0 = \frac{4}{\sqrt{2}} r = \frac{4}{\sqrt{2}} (1.43)$$

$$\boxed{a_0 = 4.04 \text{ Å}}$$

Copper is FCC and the $a_0$ to $r$ relationship is

$$a_0 = \frac{4}{\sqrt{2}} r = \frac{4}{\sqrt{2}} (1.27)$$

$$\boxed{a_0 = 3.59 \text{ Å}}$$

Magnesium is HCP and the $a_0$ to $r$ relationship is

$$a_0 = 2r$$

$$\frac{c}{a_0} = 1.633$$

$$a_0 = 2(1.6)$$

$$\boxed{a_0 = 3.2 \text{ Å}}$$

$$c = 1.633(3.2)$$

$$\boxed{c = 5.2 \text{ Å}}$$

5. Determine the crystal structure for the following: (a) a metal with a = 4.9489 Å, r = 1.75 Å, and one atom per lattice point; and (b) a metal with a = 0.42906 nm, r = 0.1858 nm and one atom per lattice point.

We want to determine if "x" in the calculations below equals 2 (for FCC) or 3 (for BCC). We know it must be one of these because we are only given $a_0$.

$$a_0 = \frac{4}{\sqrt{x}} r$$

For (a):

$$4.9489\ \text{Å} = \frac{4}{\sqrt{x}}(1.75\ \text{Å})$$

Solving:

$$x = 2$$

So the crystal is face-centered cubic (FCC)

For (b):

$$0.42906\ \text{nm} = \frac{4}{\sqrt{x}}(0.1858\ \text{nm})$$

Solving:

$$x = 3$$

So the crystal is body-centered cubic (BCC).

6. If the atomic radius of aluminum is 0.143 nm, calculate the volume of its unit cell in cubic meters. What is its coordination number and atomic packing factor? Please show your calculations.

For this problem, we are asked to calculate the volume of a unit cell of aluminum. Aluminum has an FCC crystal structure (Table 4.1). The FCC unit cell volume may be computed from Equation 4.6 as

$$V_C = 16R^3\sqrt{2} = (16)(0.143 \leftrightarrow 10^{-9}\ \text{m})^3(\sqrt{2}) = 6.62 \leftrightarrow 10^{-29}\ \text{m}^3$$

(2) The coordination number of aluminum is 12

(3) Number of atoms per unit cell of FCC is $8 \times \frac{1}{8} + 6 \times \frac{1}{6} = 4$

Atomic packing factor of FCC is $\text{APF}_{FCC} = \frac{\frac{4}{3}\pi r^3 \times 4}{a^3} = 0.74$

7. Assume that a metal exists having a simple cubic crystal structure, that is, atoms located only at the corners of a cube and touching one another along the cube edge (shown below). (a) What is the coordination number for this crystal structure? (b) Calculate the atomic packing factor.

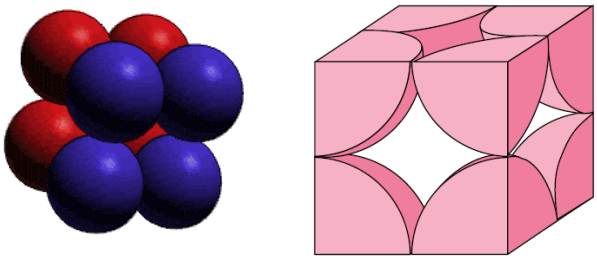


Figure 1 Simple Cubic Crystal Structure (Adapted from Callister, 5ed, Wiley)

(1) The coordination number of simple cubic is 6

(2) The number of atoms per unit cell of SC is 1

a=2r

$$APF_{SC} = \frac{\frac{4}{3}\pi r^3 \times 1}{a^3} = 0.52$$