Question #1

(i)   Explain the difference between crystal structure and atomic structure. Why is studying crystal structure important?

(ii)   Identify the closed-packed **directions** in FCC and BCC structures.

(iii)   Make a sketch for a cubic unit cell and show the $[\bar{1}\,1\,0]$, $[0\,\bar{1}\,2]$, and $[\bar{1}\,\bar{2}\,1]$ **directions.**

(iv)   Make a sketch for a cubic unit cell and show the $(0\,\bar{1}\,\bar{1})$ and $(1\,0\,\bar{2})$ **planes**.

<u>**Solution**</u>

(i)   Atomic structure relates to the number of protons and neutrons in the nucleus of an atom, as well as the number and probability distributions of the constituent electrons. On the other hand, crystal structure pertains to the arrangement of atoms in the crystalline solid material.

Study of the crystal structure is important because many material properties (especially mechanical) are determined by the arrangement of the constituent atoms.

(ii)   The closed-packed directions are the directions along which atoms are touching. For FCC and BCC the closed packed directions are <110> and <111> respectively.

(iii)   The directions asked for are indicated in the cubic unit cells shown below.
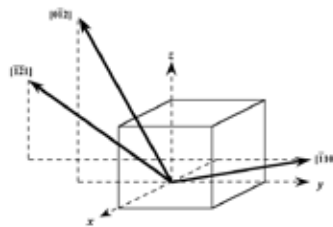

(iv)
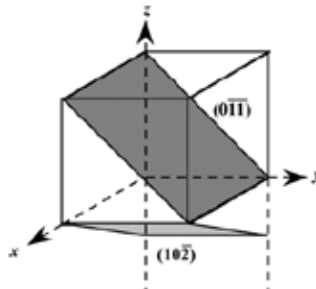
Question #2

(i)   Determine the relationship between the atomic radius, r, and lattice parameter, a, for the SC, BCC and FCC structures. If the lattice parameter of Molybdenum (Mo) is a = 3.22×10^{-10} m, calculate its atomic radius.

(ii)   Rhodium has an atomic radius of 0.1345 nm and a density of 12.41 g/cm^3. Using this information, determine whether it has an FCC or BCC crystal structure.

<u>Solution</u>

(i)
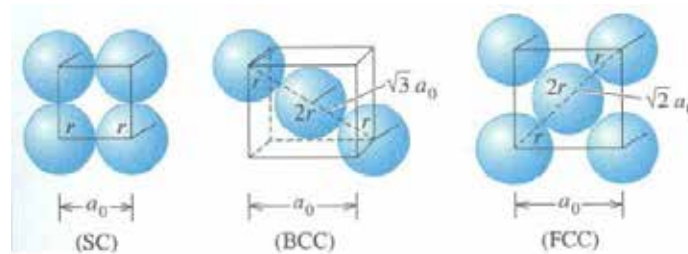
Atoms touch along the edge of the cube in SC structures and $a_0 = 2r$.
In BCC structures, atoms touch along the body diagonal, which is $\sqrt{3}$ a. So, $a_0 = 4r/\sqrt{3}$
In FCC structures, atoms touch along the face diagonal of the cube, which is $\sqrt{2}$ a. So, $a_0 = 4r/\sqrt{2}$

Since Mo is a BCC material, the relation between atomic radius and lattice parameter for BCC materials is as follows:

$$\text{For BCC, } a\sqrt{3} = 4r \text{ , so } r = 1.39 \times 10^{-10} \text{ m}$$

(ii)   The atomic weight is 102.91 g/mol.

In order to determine whether Rh has an FCC or a BCC crystal structure, we need to compute its density for each of the crystal structures. First, we will assume that Rh has an FCC structure. So, for FCC, $n = 4$ and the lattice parameter is $a = 2R\sqrt{2}$. So, employing equation 3.5,

$$\rho = \frac{n A_{Rh}}{a^3 N_A} = \frac{n A_{Rh}}{(2R\sqrt{2})^3 N_A}$$

$$= \frac{(4 \text{ atoms/unit cell})(102.91 \text{ g/mol})}{\left\{ \left[(2)(1.345 \times 10^{-8} \text{ cm})(\sqrt{2}) \right]^3 /(\text{unit cell}) \right\}(6.022 \times 10^{23} \text{ atoms/mol})}$$

$$= 12.41 \text{ g/cm}^3$$

which is the value provided in the problem statement. Therefore, Rh has the FCC crystal

structure

Question #3

   (i)   Calculate the **highest** linear density (atoms/m) encountered in Vanadium (V).

   (ii)   For Vanadium, calculate the planar density value for the (100) plane.

Solution

   (i)   From the tables, we know that V is a BCC material and its atomic weight and density

          of V are as follows

          V: atomic weight = 50.94 g/mole

                 $\rho = 5.8$ g/cm^3

          BCC, so n = 2

          The highest density would be found in the [111] direction. To find "a":

          $$\frac{\text{atomic weight}}{\rho} = a^3 \frac{N_A}{n} \rightarrow a^3 = \frac{50.94 \times 2}{5.8 \times 6.023 \times 10^{23}}$$
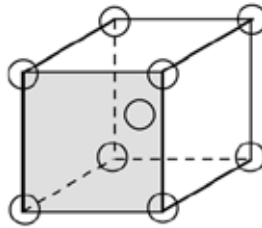
          $a = 3.08 \times 10^{-8}$ cm $= 3.08 \times 10^{-10}$ m

          The length in the [111] direction is $a\sqrt{3}$, so there are:

          2 atoms / $a\sqrt{3}$ = 2 atoms/$(3.08 \times 10^{-10}$ m $\times \sqrt{3})$

          = 3.75 x 10^9 atoms/m

   (ii)   Since V has a BCC unit cell. The (100) plane is shown below.

The planar density is:

$$PD_{100} = \frac{\text{number of atoms centered on (100) plane}}{\text{area of (100) plane}}$$

For this (100) plane there is one atom at each of the four cube corners, each of which is shared

with four adjacent unit cells. Thus, there is the equivalence of 1 atom associated with this BCC

(100) plane.

The planar section represented in the above figure is a square, wherein the side lengths are equal to the unit cell edge length (the lattice parameter), $\frac{4R}{\sqrt{3}}$. The area of this square is then,

$$\left(\frac{4R}{\sqrt{3}}\right)^2 = \frac{16R^2}{3}$$

And the planar density is,

$$= \frac{1\ \text{atom}}{\dfrac{16\ R^2}{3}} = \frac{3}{16\ R^2}$$

$$= \frac{3}{16\,(0.132\ \text{nm})^2} = 10.76\ \text{nm}^{-2} = 1.076 \times 10^{19}\ \text{m}^{-2}$$

Question #4

(i)   Calculate the interplanar spacing (d_{hkl}) of {1 1 0} planes in Copper (Cu), where the lattice parameter is $a = 3.61 \times 10^{-10}$ m.

(ii) Determine the expected diffraction angle (2θ) for the first-order reflection from the (1 1 3) set of planes for FCC platinum when monochromatic radiation of wavelength 0.1542 nm is used. The atomic radius of platinum is 0.1387 nm.

Solution

(i)

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$d_{110} = \frac{3.61 \times 10^{-10}}{\sqrt{2}} = 2.55 \times 10^{-10} \text{ m}$$

(iii) From the atomic radius we can calculate the lattice parameter as follows

$$a = 2R\sqrt{2} = (2)(0.1387 \text{ nm})(\sqrt{2}) = 0.3923 \quad \text{nm}$$

The interplanar spacing can then be calculated using

$$d_{(hkl)} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$d_{113} = \frac{a}{\sqrt{(1)^2 + (1)^2 + (3)^2}} = \frac{0.3923 \text{ nm}}{\sqrt{11}} = 0.1183 \quad \text{nm}$$

Now, Bragg's can be used to calculate the diffraction angle,

$$\sin \theta = \frac{n\lambda}{2d_{113}} = \frac{(1)(0.1542 \text{ nm})}{(2)(0.1183 \text{ nm})} = 0.652$$

Which leads to

$$\theta = \sin^{-1}(0.652) = 40.69°$$

And, finally

$$2\theta = (2)(40.69°) = 81.38°$$