HW #2

3.2 *If the atomic radius of aluminum is 0.143 nm, calculate the volume of its unit cell in cubic meters.*
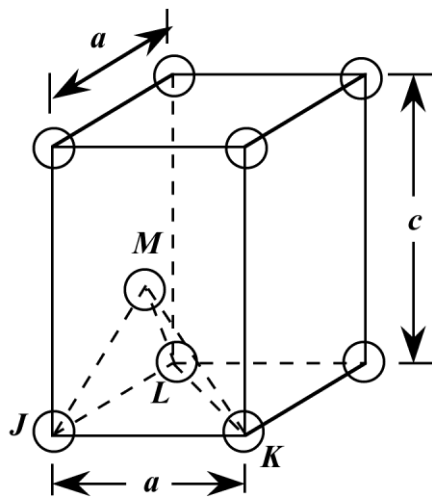
Solution

For this problem, we are asked to calculate the volume of a unit cell of aluminum. Aluminum has an FCC crystal structure (Table 3.1). The FCC unit cell volume may be computed from Equation 3.4 as

$$V_C = 16R^3\sqrt{2} = (16)(0.143 \times 10^{-9} \text{ m})^3(\sqrt{2}) = 6.62 \times 10^{-29} \text{ m}^3$$
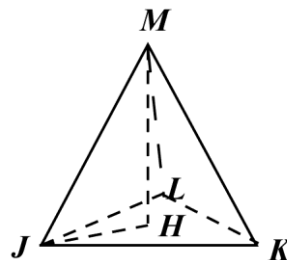
3.4 *For the HCP crystal structure, show that the ideal c/a ratio is 1.633.*

Solution

A sketch of one-third of an HCP unit cell is shown below.

Consider the tetrahedron labeled as *JKLM*, which is reconstructed as

The atom at point M is midway between the top and bottom faces of the unit cell--that is $\overline{MH} = c/2$. And, since atoms at points J, K, and M, all touch one another,

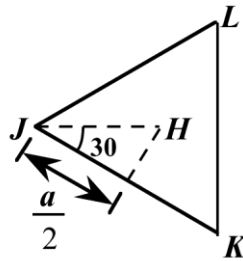$$\overline{JM} = \overline{JK} = 2R = a$$

where R is the atomic radius. Furthermore, from triangle JHM,

$$(\overline{JM})^2 = (\overline{JH})^2 + (\overline{MH})^2$$

or

$$a^2 = (\overline{JH})^2 + \left(\frac{c}{2}\right)^2$$

Now, we can determine the $\overline{JH}$ length by consideration of triangle JKL, which is an equilateral triangle,

$$\cos 30° = \frac{a/2}{JH} = \frac{\sqrt{3}}{2}$$

and

$$\overline{JH} = \frac{a}{\sqrt{3}}$$

Substituting this value for $\overline{JH}$ in the above expression yields

$$a^2 = \left(\frac{a}{\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)^2 = \frac{a^2}{3} + \frac{c^2}{4}$$

and, solving for c/a

$$\frac{c}{a} = \sqrt{\frac{8}{3}} = 1.633$$

3.9 *Calculate the radius of a vanadium atom, given that V has a BCC crystal structure, a density of 5.96 g/cm³, and an atomic weight of 50.9 g/mol.*

<u>Solution</u>

This problem asks for us to calculate the radius of a vanadium atom. For BCC, $n = 2$ atoms/unit cell, and

$$V_C = \left(\frac{4R}{\sqrt{3}}\right)^3 = \frac{64R^3}{3\sqrt{3}}$$

Since, from Equation 3.5

$$\rho = \frac{nA_V}{V_C N_A}$$

$$= \frac{nA_V}{\left(\dfrac{64R^3}{3\sqrt{3}}\right)N_A}$$

and solving for R the previous equation

$$R = \left(\frac{3\sqrt{3}nA_V}{64\,\rho\,N_A}\right)^{1/3}$$

and incorporating values of parameters given in the problem statement

$$R = \left[\frac{\left(3\sqrt{3}\right)(2 \text{ atoms/unit cell})(50.9 \text{ g/mol})}{(64)\left(5.96 \text{ g/cm}^3\right)\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}\right]^{1/3}$$

$$= 1.32 \times 10^{-8} \text{ cm} = 0.132 \text{ nm}$$

3.13 *Rhodium has an atomic radius of 0.1345 nm and a density of 12.41 g/cm³. Determine whether it has an FCC or BCC crystal structure.*

Solution

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. For FCC, $n = 4$, and $a = 2R\sqrt{2}$ (Equation 3.1). Also, from Figure 2.6, its atomic weight is 102.91 g/mol. Thus, for FCC (employing Equation 3.5)

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

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

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

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

3.14 *Below are listed the atomic weight, density, and atomic radius for three hypothetical alloys. For each determine whether its crystal structure is FCC, BCC, or simple cubic and then justify your determination. A simple cubic unit cell is shown in Figure 3.24.*

Alloy	Atomic Weight (g/mol)	Density (g/cm³)	Atomic Radius (nm)
A	77.4	8.22	0.125
B	107.6	13.42	0.133
C	127.3	9.23	0.142

Solution

For each of these three alloys we need, by trial and error, to calculate the density using Equation 3.5, and compare it to the value cited in the problem. For SC, BCC, and FCC crystal structures, the respective values of n are 1, 2, and 4, whereas the expressions for a (since $V_C = a^3$) are $2R$, $2R\sqrt{2}$, and $\frac{4R}{\sqrt{3}}$.

For alloy A, let us calculate ρ assuming a simple cubic crystal structure.

$$\rho = \frac{nA_A}{V_C N_A}$$

$$= \frac{nA_A}{(2R)^3 N_A}$$

$$= \frac{(1 \text{ atom/unit cell})(77.4 \text{ g/mol})}{\left\{\left[(2)(1.25 \times 10^{-8})\right]^3/(\text{unit cell})\right\}(6.022 \times 10^{23} \text{ atoms/mol})}$$

$$= 8.22 \text{ g/cm}^3$$

Therefore, its crystal structure is simple cubic.

For alloy B, let us calculate ρ assuming an FCC crystal structure.

$$\rho = \frac{nA_B}{(2R\sqrt{2})^3 N_A}$$

$$= \frac{(4 \text{ atoms/unit cell})(107.6 \text{ g/mol})}{\left\{\left[(2\sqrt{2})(1.33 \times 10^{-8} \text{ cm})\right]^3/(\text{unit cell})\right\}(6.022 \times 10^{23} \text{ atoms/mol})}$$

$$= 13.42 \text{ g/cm}^3$$

Therefore, its crystal structure is FCC.

For alloy C, let us calculate ρ assuming a simple cubic crystal structure.

$$= \frac{nA_C}{(2R)^3 N_A}$$

$$= \frac{(1 \text{ atom/unit cell})(127.3 \text{ g/mol})}{\left\{\left[(2)(1.42 \times 10^{-8} \text{ cm})\right]^3/(\text{unit cell})\right\}(6.022 \times 10^{23} \text{ atoms/mol})}$$

$$= 9.23 \text{ g/cm}^3$$

Therefore, its crystal structure is simple cubic.