Metals:

It's a material in which the valence electrons are detached from atoms, and spread in an 'electron sea' that "glues" the ions together. Strong, ductile, conduct electricity and heat well, are shiny if polished. Examples of metals are gold, aluminium, iron and magnesium etc.

They show the following properties .Physical Properties of Metals: Some of the main physical properties of metals are given below.

1.Metals can be hammered into thin sheets. It means they possess the property of malleability.

2.Metals are ductile. They can be drawn into wires.

3.Metals are a good conductor of heat and electricity.

4. Metals are lustrous which means they have a shiny appearance.

5. Metals have high tensile strength. It means they can hold heavyweights.

6. Metals are sonorous. It means when we strike them, they make a ringing sound.

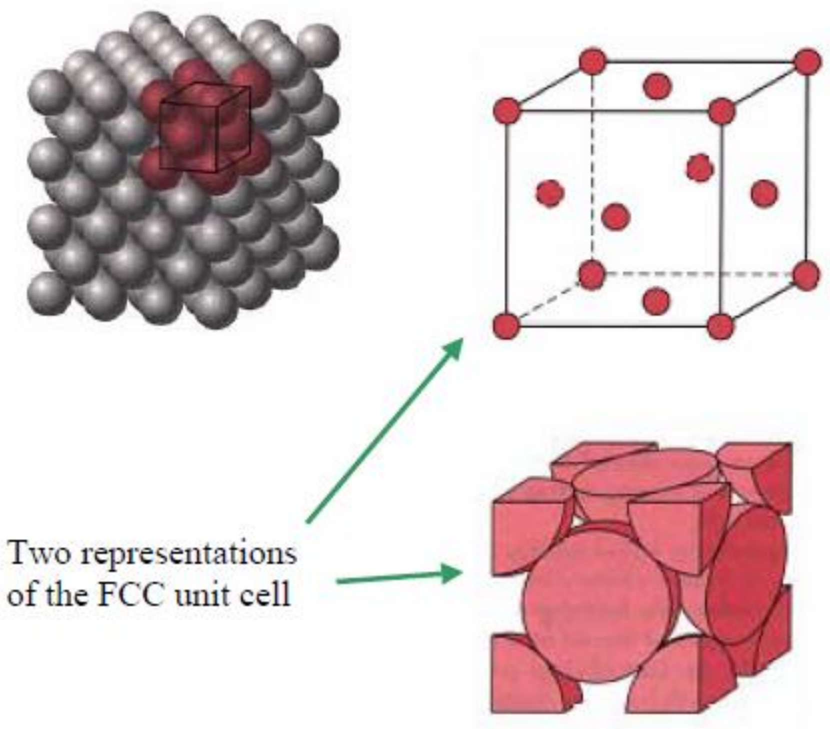
7. Metals are hard. It means they cannot be cut easily.

METALLIC CRYSTAL STRUCTURES

The atomic bonding in this group of materials is metallic, and thus nondirectional in nature. Consequently, there are no restrictions as to the number and position of nearest-neighbor atoms; this leads to relatively large numbers of nearest neighbors and dense atomic packings for most metallic crystal structures. Three relatively simple crystal structures are found for most of the common metals: face-centered cubic, body-centered cubic, and hexagonal close-packed

1. THE FACE-CENTERED CUBIC CRYSTAL STRUCTURE

The crystal structure found for many metals has a unit cell of cubic geometry, with atoms located at each of the corners and the centers of all the cube faces. It is aptly called the face-centered cubic (FCC) crystal structure. Some of the familiar metals having this crystal structure are copper, aluminum, silver, and gold. Figure 3.1 Shaw a hard sphere model for the FCC unit cell, whereas in Figure 3.1b the atom centers are represented by small circles to provide a better perspective of atom positions. The aggregate of atoms in Figure 3.1c represents a section of crystal consisting of many FCC unit cells. These spheres or ion cores touch one another across a face diagonal; the cube edge length a and the atomic radius R are related through



$$a = 2R\sqrt{2}$$

For the FCC crystal structure, each corner atom is shared among eight unit cells, whereas a face-centered atom belongs to only two.

Two other important characteristics of a crystal structure are the coordination number and For metals, each atom has the same number of nearest-neighbor or touching atoms, which is the coordination number. For face-centered cubics, the coordination number is 12. This may be confirmed by examination of Figure 3.1a; the front face atom has four corner nearest-neighbor atoms surrounding it, four face atoms that are in contact from behind, and four other equivalent face atoms residing in the next unit cell to the front, which is not shown.

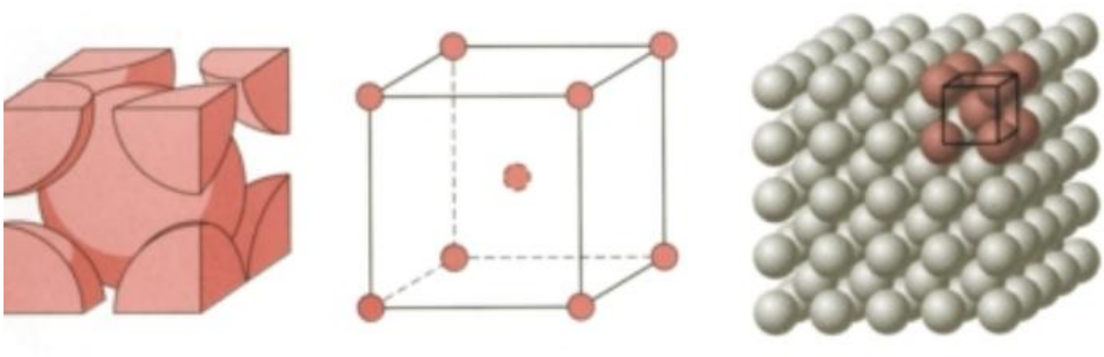
The APF is the fraction of solid sphere volume in a unit cell, assuming the atomic hard sphere model, or

APF = volume of atoms in a unit cell/ total unit cell volume

For the FCC structure, the atomic packing factor is 0.74, which is the maximum packing possible for spheres all having the same diameter. Computation of this APF is also included as an example problem.

2.THE BODY-CENTERED CUBIC CRYSTAL STRUCTURE:

Another common metallic crystal structure also has a cubic unit cell with atoms located at all eight corners and a single atom at the cube center. This is called a body-centered cubic (BCC) crystal structure. A collection of spheres depicting this crystal structure is shown in Figure 3.2c, whereas Figures 3.2a and 3.2b are diagrams



(a) (b) (c)

FIGURE 3.2 For the body-centered cubic crystal structure, (*a*) a hard sphere unit cell representation, (*b*) a reduced-sphere unit cell, and (*c*) an aggregate of many atoms. (Figure (*c*) from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. I, *Structure*, p. 51. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)

of BCC unit cells with the atoms represented by hard sphere and reduced-sphere models, respectively. Center and corner atoms touch one another along cube diagonals, and unit cell length a and atomic radius R are related through a

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

The coordination number for the BCC crystal structure is 8; each center atom has as nearest neighbors its eight corner atoms. Since the coordination number is less for BCC than FCC, so also is the atomic packing factor for BCC lower—0.68 versus 0.74.

3.THE HEXAGONAL CLOSE-PACKED CRYSTAL STRUCTURE:

Not all metals have unit cells with cubic symmetry; the final common metallic crystal structure to be discussed has a unit cell that is hexagonal. Figure 3.3a shows a reduced-sphere unit cell for this structure, which is termed hexagonal close-packed (HCP); an assemblage of several HCP unit cells is presented in Figure 3.3b. The top and bottom faces of the unit cell consist of six atoms that form regular hexagons and surround a single atom in the center. Another plane that provides three additional atoms to the unit cell is situated between the top and bottom planes. The atoms in this midplane have as nearest neighbors atoms in both of the adjacent two planes. The equivalent of six atoms is contained in each unit cell; one-sixth of each of the 12 top and bottom face corner atoms, one-half of each of the 2 center face atoms, and all the 3 midplane interior atoms. If a and c represent, respectively

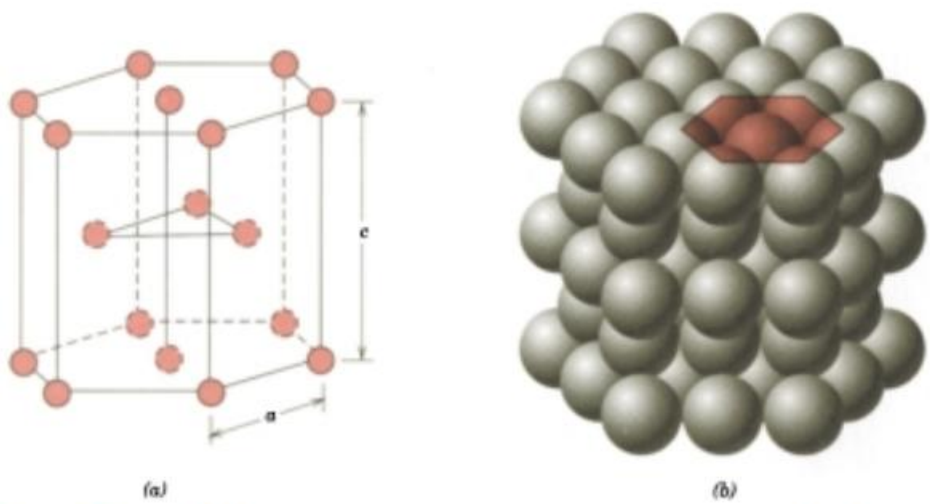


FIGURE 3.3 For the hexagonal close-packed crystal structure, (*a*) a reduced-sphere unit cell (*a* and *c* represent the short and long edge lengths, respectively), and (*b*) an aggregate of many atoms. (Figure (*b*) from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials,* Vol. I, *Structure,* p. 51. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)

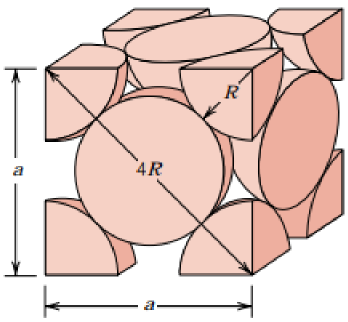
he short and long unit cell dimensions of Figure 3.3a, the c/a ratio should be 1.633; however, for some HCP metals this ratio deviates from the ideal value. The coordination number and the atomic packing factor for the HCP crystal structure are the same as for FCC: 12 and 0.74, respectively. The HCP metals include cadmium, magnesium, titanium, and zinc

EXAMPLE PROBLEM 3.1

Calculate the volume of an FCC unit cell in terms of the atomic radius R.

SOLUTION

In the FCC unit cell illustrated,



the atoms touch one another across a face-diagonal the length of which is $4R$. Since the unit cell is a cube, its volume is a^3, where a is the cell edge length. From the right triangle on the face,

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

or, solving for a,

$$a = 2R\sqrt{2} \quad (3.1)$$

The FCC unit cell volume V_C may be computed from

$$V_C = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2} \quad (3.4)$$

Number of atoms per unit cell, n = 4. (For an atom that is shared with m adjacent unit cells, we only count a fraction of the atom, 1/m). In FCC unit cell we have:

6 face atoms shared by two cells: 6 x 1/2 = 3

8 corner atoms shared by eight cells: 8 x 1/8 = 1

3.5 Density Computations—Metals

A knowledge of the crystal structure of a metallic solid permits computation of its theoretical density ρ through the relationship

$$\rho = \frac{nA}{V_C N_A} \tag{3.5}$$

where

n = number of atoms associated with each unit cell

A = atomic weight

V_C = volume of the unit cell

N_A = Avogadro's number (6.023×10^{23} atoms/mol)

Example Problem 3.3

Copper has an atomic radius of 0.128 nm (1.28 Å), an FCC crystal structure, and an atomic weight of 63.5 g/mol. Compute its theoretical density and compare the answer with its measured density.

Solution

Equation 3.5 is employed in the solution of this problem. Since the crystal structure is FCC, n, the number of atoms per unit cell, is 4. Furthermore, the atomic weight A_{Cu} is given as 63.5 g/mol. The unit cell volume V_C for FCC was determined in Example Problem 3.1 as $16R^3\sqrt{2}$, where R, the atomic radius, is 0.128 nm.

Substitution for the various parameters into Equation 3.5 yields

$$\rho = \frac{nA_{Cu}}{V_C N_A} = \frac{nA_{Cu}}{(16R^3\sqrt{2})\,N_A}$$

$$= \frac{(4\ \text{atoms/unit cell})(63.5\ \text{g/mol})}{[16\sqrt{2}(1.28 \times 10^{-8}\ \text{cm})^3/\text{unit cell}](6.023 \times 10^{23}\ \text{atoms/mol})}$$

$$= 8.89\ \text{g/cm}^3$$

The literature value for the density of copper is 8.94 g/cm^3, which is in very close agreement with the foregoing result.

Example Problem 3.2

Show that the atomic packing factor for the FCC crystal structure is 0.74.

Solution

The APF is defined as the fraction of solid sphere volume in a unit cell, or

$$\text{APF} = \frac{\text{total sphere volume}}{\text{total unit cell volume}} = \frac{V_S}{V_C}$$

Both the total sphere and unit cell volumes may be calculated in terms of the atomic radius R. The volume for a sphere is $\frac{4}{3}\pi R^3$, and since there are four

atoms per FCC unit cell, the total FCC sphere volume is

$$V_S = (4)\frac{4}{3}\pi R^3 = \frac{16}{3}\pi R^3$$

From Example Problem 3.1, the total unit cell volume is

$$V_C = 16R^3\sqrt{2}$$

Therefore, the atomic packing factor is

$$\text{APF} = \frac{V_S}{V_C} = \frac{(\frac{16}{3})\pi R^3}{16R^3\sqrt{2}} = 0.74$$