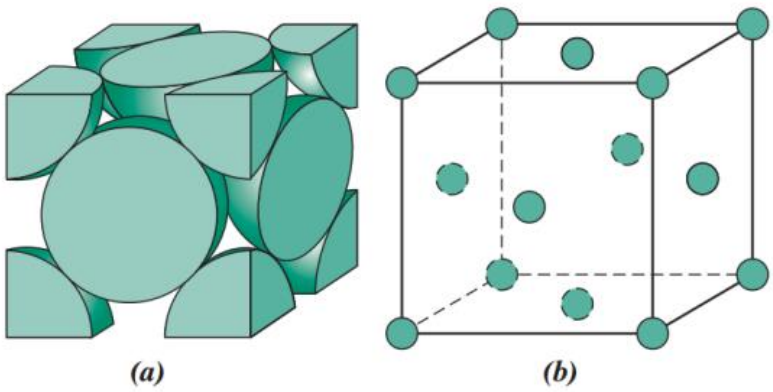
The Face-Centered Cubic Crystal Structure

The cube edge length a and the atomic radius (R) are related through

Table 3.1
Atomic Radii and Crystal Structures for 16 Metals

Metal	*Crystal Structure*[a]	*Atomic Radius*[b] *(nm)*	*Metal*	*Crystal Structure*	*Atomic Radius (nm)*
Aluminum	FCC	0.1431	Molybdenum	BCC	0.1363
Cadmium	HCP	0.1490	Nickel	FCC	0.1246
Chromium	BCC	0.1249	Platinum	FCC	0.1387
Cobalt	HCP	0.1253	Silver	FCC	0.1445
Copper	FCC	0.1278	Tantalum	BCC	0.1430
Gold	FCC	0.1442	Titanium (α)	HCP	0.1445
Iron (α)	BCC	0.1241	Tungsten	BCC	0.1371
Lead	FCC	0.1750	Zinc	HCP	0.1332

[a]FCC = face-centered cubic; HCP = hexagonal close-packed; BCC = body-centered cubic.
[b]A nanometer (nm) equals 10^{-9} m; to convert from nanometers to angstrom units (Å), multiply the nanometer value by 10.



(a) *(b)*

The number of atoms per unit cell, N, can be computed using the following formula:

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8} \qquad *$$

Where

N_i: the number of interior atoms,

N_f: the number of face atoms,

N_c: the number of corner atoms.

For the FCC crystal structure, there are eight corner atoms ($N_c = 8$), six face atoms ($N_f = 6$), and no interior atoms ($N_i = 0$). Thus, from Equation above,

$$N = 0 + \frac{6}{2} + \frac{8}{8} = 0 + 3 + 1 = 4$$

Atomic packing factor (APF) عامل التعبئه الذري

The APF is the sum of the sphere volumes of all atoms within a unit cell (assuming the atomic hard-sphere model) divided by the unit cell volume—that is,

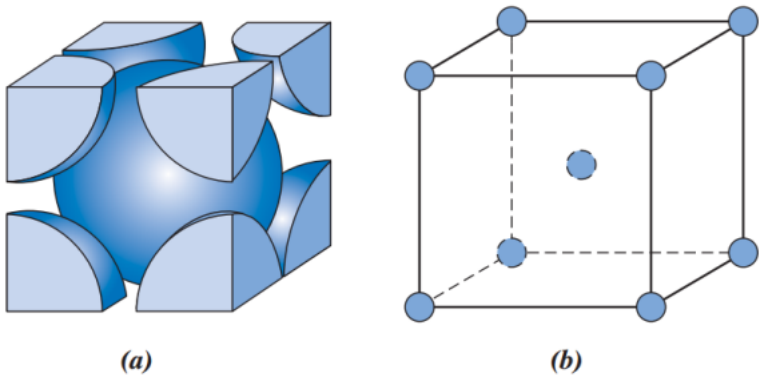
$$APF = \frac{Volume\ of\ \ atoms\ in\ a\ unit\ cell}{total\ unit\ cell\ volume}$$

For the FCC structure, the atomic packing factor is 0.74, which is the maximum packing possible for spheres all having the same diameter.

coordination number

The face-centered cubic (FCC) has a coordination number of 12 and contains 4 atoms per unit cell. The body-centered cubic (BCC) has a coordination number of 8 and contains 2 atoms per unit cell. The simple cubic has a coordination number of 6 and contains 1 atom per unit cell.

The Body-Centered Cubic Crystal Structure



(a) (b)

Center and corner atoms touch one another along cube diagonals, and unit cell length a and atomic radius (R) are related through

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

the number of atoms per BCC unit cell is

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$
$$= 1 + 0 + \frac{8}{8} = 2$$

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

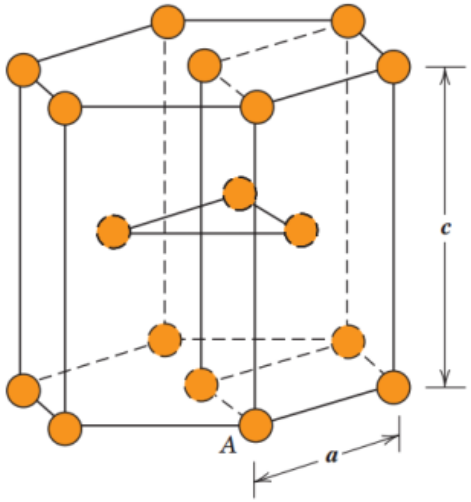
The Hexagonal Close-Packed Crystal Structure

In order to compute the number of atoms per unit cell for the HCP crystal structure, Equation * is modified to read as follows:

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{6}$$

That is, one-sixth of each corner atom is assigned to a unit cell (instead of 8 as with the cubic structure). Because for HCP there are 6 corner atoms in each of the top and bottom faces (for a total of 12 corner atoms), 2 face center atoms (one from each of the top and bottom faces), and 3 midplane interior atoms, the value of N for HCP is found, using Equation above, to be

$$N = 3 + \frac{2}{2} + \frac{12}{6}$$



The coordination number and the atomic packing factor for the HCP crystal structure are the same as for FCC: 12 and 0.74.

EXAMPLE PROBLEM 3.1

Determination of FCC Unit Cell Volume

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 $4R$. Because 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,

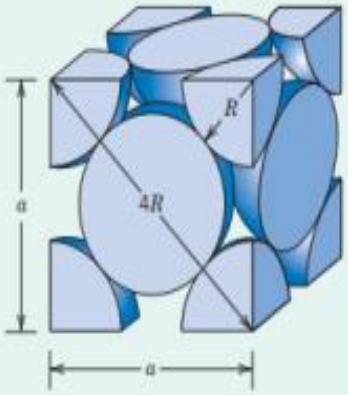
$$a^2 + a^2 = (4R)^2$$

or, solving for a,

$$a = 2R\sqrt{2} \tag{3.1}$$

The FCC unit cell volume V_C may be computed from

$$V_C = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2} \tag{3.6}$$



EXAMPLE PROBLEM 3.2

Computation of the Atomic Packing Factor for FCC

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

$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}} = \frac{V_S}{V_C}$$

Both the total atom 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 because there are four atoms per FCC unit cell, the total FCC atom (or sphere) volume is

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

From Example Problem 3.1, the total unit cell volume is

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

Therefore, the atomic packing factor is

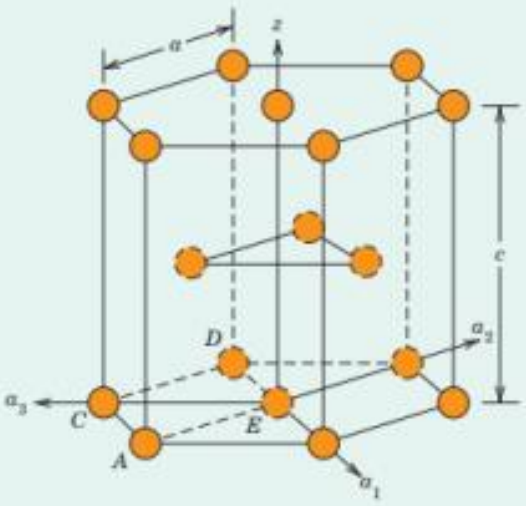
$$\text{APF} = \frac{V_S}{V_C} = \frac{\left(\frac{16}{3}\right)\pi R^3}{16R^3\sqrt{2}} = 0.74$$

EXAMPLE PROBLEM 3.3

Determination of HCP Unit Cell Volume

(a) Calculate the volume of an HCP unit cell in terms of its a and c lattice parameters.

(b) Now provide an expression for this volume in terms of the atomic radius, R, and the c lattice parameter.

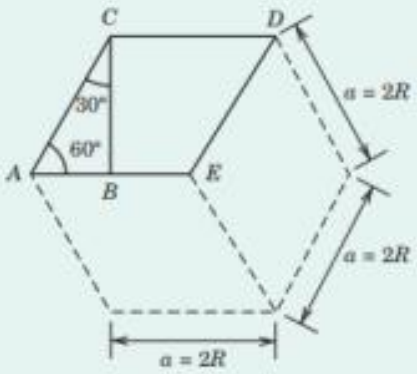


Solution

(a) We use the adjacent reduced-sphere HCP unit cell to solve this problem.

Now, the unit cell volume is just the product of the base area times the cell height, c. This base area is just three times the area of the parallelepiped $ACDE$ shown below. (This $ACDE$ parallelepiped is also labeled in the above unit cell.)

The area of $ACDE$ is just the length of $\overline{CD}$ times the height $\overline{BC}$. But $\overline{CD}$ is just a, and $\overline{BC}$ is equal to



$$\overline{BC} = a\cos(30°) = \frac{a\sqrt{3}}{2}$$

Thus, the base area is just

$$\text{AREA} = (3)(\overline{CD})(\overline{BC}) = (3)(a)\left(\frac{a\sqrt{3}}{2}\right) = \frac{3a^2\sqrt{3}}{2}$$

Again, the unit cell volume V_C is just the product of the AREA and c; thus,

$$\begin{aligned} V_C &= \text{AREA}(c) \\ &= \left(\frac{3a^2\sqrt{3}}{2}\right)(c) \\ &= \frac{3a^2c\sqrt{3}}{2} \end{aligned} \tag{3.7a}$$

(b) For this portion of the problem, all we need do is realize that the lattice parameter a is related to the atomic radius R as

$$a = 2R$$

Now making this substitution for a in Equation 3.7a gives

$$\begin{aligned} V_C &= \frac{3(2R)^2c\sqrt{3}}{2} \\ &= 6R^2c\sqrt{3} \end{aligned} \tag{3.7b}$$

DENSITY COMPUTATIONS:

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

$$\rho = \frac{n A}{V_C N_A}$$

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 (6.022×10^{23} atoms/mol)

EXAMPLE PROBLEM 3.4

Theoretical Density Computation for Copper

Copper has an atomic radius of 0.128 nm, 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 3.8 is employed in the solution of this problem. Because 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 3.8 yields

$$\begin{aligned}\rho_{Cu} &= \frac{nA_{Cu}}{V_C N_A} = \frac{nA_{Cu}}{(16R^3\sqrt{2})N_A} \\ &= \frac{(4 \text{ atoms/unit cell})(63.5 \text{ g/mol})}{[16\sqrt{2}(1.28 \times 10^{-8} \text{ cm})^3/\text{unit cell}](6.022 \times 10^{23} \text{ atoms/mol})} \\ &= 8.89 \text{ g/cm}^3\end{aligned}$$

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