Materials Science: The Structure of Solids, Crystal Structure, BCC, CPH (Week 5)

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The Body- Centred 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 centre. This is called a body-centred 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 of BCC unit cells with the atoms represented by hard-sphere and reduced-sphere models, respectively.

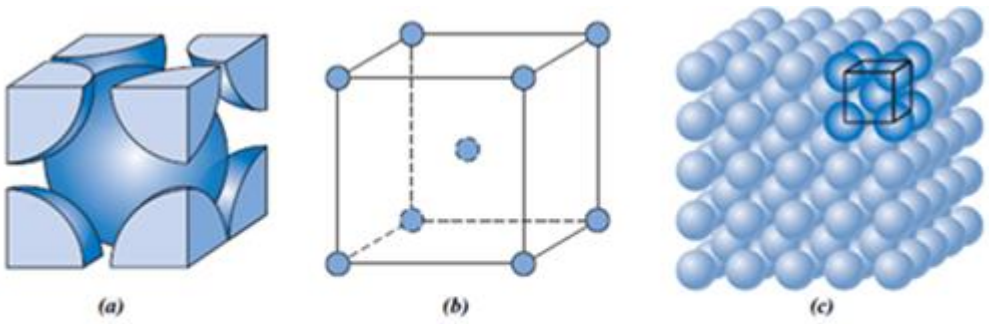
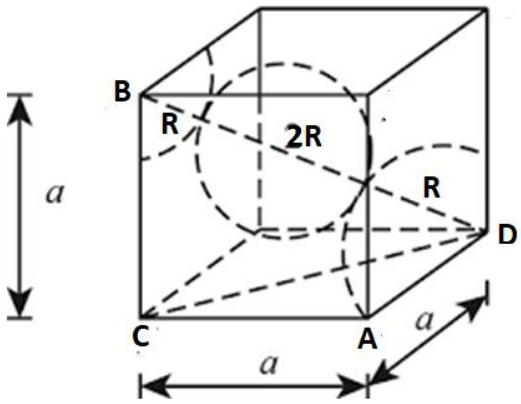


Figure 3.2 For the body-centred cubic crystal structure, (a) a hard-sphere unit cell representation, (b) a reduced sphere unit cell, and (c) an aggregate of many atoms.

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

$$a = \frac{4R}{\sqrt{3}} \qquad (3.4)$$



Chromium, iron, tungsten, and several other metals listed in Table 3.1 exhibit a BCC structure.

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.

Each BCC unit cell has eight corner atoms and a single center atom, which is wholly contained within its cell; therefore, from Equation 3.2, 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.

$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}} \qquad (3.3)$$

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 3.4a 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 3.4b. 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 mid plane have as nearest neighbors' atoms in both of the adjacent two planes.

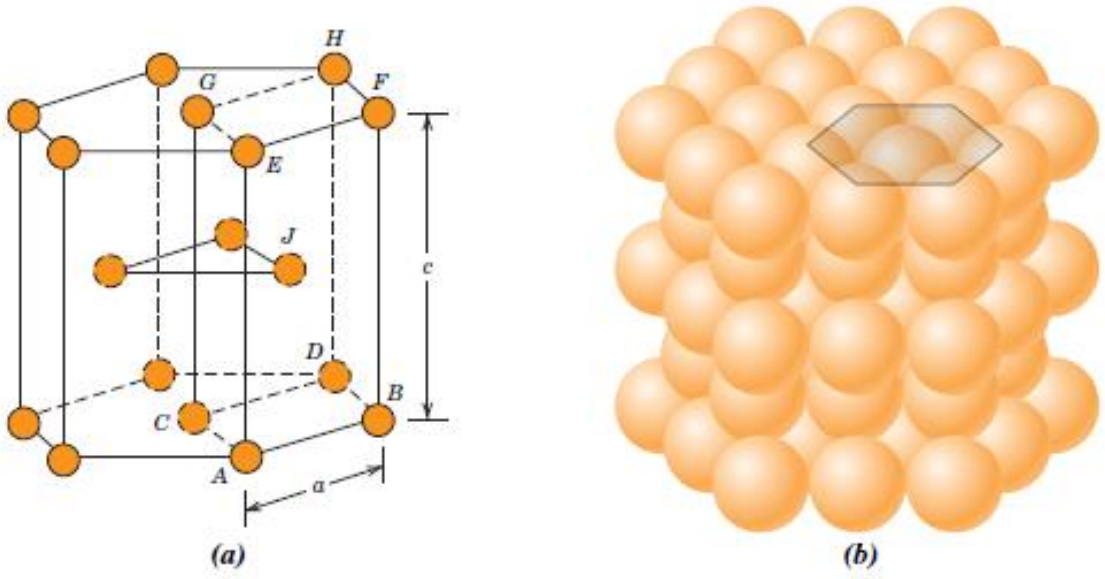


Figure 3.4 For the hexagonal close-packed crystal structure, (a) a reduced-sphere unit cell [(a) and (c) represent the short and long edge lengths, respectively), and (b) an aggregate of many atoms.

In order to compute the number of atoms per unit cell for the HCP crystal structure, Equation 3.2 is modified to read as follows:

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{6} \tag{3.5}$$

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 mid plane interior atoms, the value of N for HCP is found, using Equation 3.5, to be

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

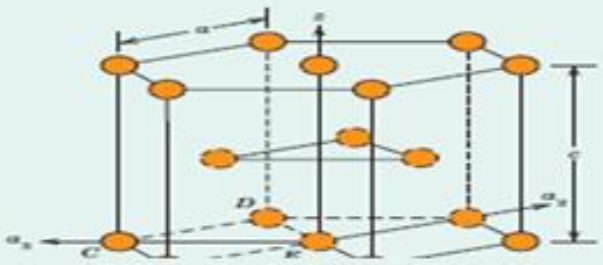
Thus, 6 atoms are assigned to each unit cell.

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.

Thus, the base area is just

$$\text{AREA} = \frac{3a^2\sqrt{3}}{2}$$

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

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

(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

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

3.6 POLYMORPHISM AND ALLOTROPY

Some metals, as well as non metals, may have more than one crystal structure, a phenomenon known as polymorphism. When found in elemental solids, the condition is often termed allotropy. One familiar example is found in carbon: graphite is the stable polymorph at ambient conditions, whereas diamond is formed at extremely high pressures. Also, pure iron has a BCC crystal structure at room temperature, which changes to FCC iron at 912°C (1674°F).

Another common metal that experiences an allotropic change is White (β) tin., having a body-centered tetragonal crystal structure at room temperature, transforms, at 13.2°C (55.8°F), to Gray (α) , which has a crystal structure similar to that of diamond (i.e., the diamond cubic crystal structure); this transformation is represented schematically as follows

