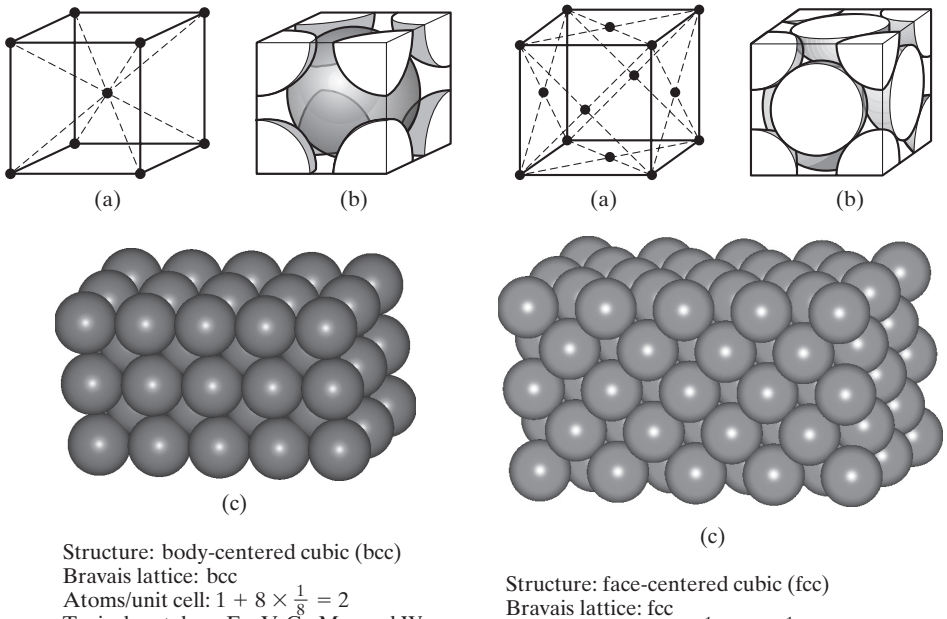
3.2 Metal Structures

With the structural ground rules behind us, we can now list the main crystal structures associated with important engineering materials. For our first group, the metals, this list is fairly simple. As we see from an inspection of Appendix 1, most elemental metals at room temperature are found in one of three crystal structures.

Figure 3.4 shows the **body-centered cubic** (bcc) structure, which is the body-centered cubic **Bravais lattice** with one atom centered on each lattice point. There is one atom at the center of the unit cell and one-eighth atom at each of eight unit-cell corners. (Each corner atom is shared by eight adjacent unit cells.) Thus, there are two atoms in each bcc unit cell. The **atomic packing factor (APF)** for this structure is 0.68 and represents the fraction of the unit-cell volume occupied by the two atoms. Typical metals with this structure include α-Fe (the form stable at room temperature), V, Cr, Mo, and W. An alloy in which one of these metals is the predominant constituent will tend to have this structure also. However, the presence of alloying elements diminishes crystalline perfection, a topic that will be discussed in Chapter 4.

Figure 3.5 shows the **face-centered cubic** (fcc) structure, which is the fcc Bravais lattice with one atom per lattice point. There is one-half atom (i.e., one atom shared between two unit cells) in the center of each unit-cell face and one-eighth atom at each unit-cell corner, for a total of four atoms in each fcc unit cell. The atomic packing factor for this structure is 0.74, a value slightly higher than the 0.68 found for bcc metals. In fact, an APF of 0.74 is the highest value possible for filling space by stacking equal-sized hard spheres. For this reason, the fcc structure is sometimes referred to as **cubic close packed** (ccp). Typical metals with the fcc structure include γ-Fe (stable from 912 to 1,394°C), Al, Ni, Cu, Ag, Pt, and Au.



Structure: body-centered cubic (bcc)
Bravais lattice: bcc
Atoms/unit cell: $1 + 8 \times \frac{1}{8} = 2$
Typical metals: α-Fe, V, Cr, Mo, and W

FIGURE 3.4 *Body-centered cubic (bcc) structure for metals showing (a) the arrangement of lattice points for a unit cell, (b) the actual packing of atoms (represented as hard spheres) within the unit cell, and (c) the repeating bcc structure, equivalent to many adjacent unit cells. [Part (c) courtesy of Accelrys, Inc.]*

Structure: face-centered cubic (fcc)
Bravais lattice: fcc
Atoms/unit cell: $6 \times \frac{1}{2} + 8 \times \frac{1}{8} = 4$
Typical metals: γ-Fe, Al, Ni, Cu, Ag, Pt, and Au

FIGURE 3.5 *Face-centered cubic (fcc) structure for metals showing (a) the arrangement of lattice points for a unit cell, (b) the actual packing of atoms within the unit cell, and (c) the repeating fcc structure, equivalent to many adjacent unit cells. [Part (c) courtesy of Accelrys, Inc.]*

The **hexagonal close-packed** (hcp) structure (Figure 3.6) is our first encounter with a structure more complicated than its Bravais lattice (hexagonal). There are two atoms associated with each Bravais lattice point. There is one atom centered within the unit cell and various fractional atoms at the unit-cell corners (four $\frac{1}{6}$ atoms and four $\frac{1}{12}$ atoms), for a total of two atoms per unit cell. As the *close-packed* name implies, this structure is as efficient in packing spheres as is the fcc structure. Both hcp and fcc structures have atomic packing factors of 0.74, which raises two questions: (1) In what other ways are the fcc and hcp structures alike? and (2) How do they differ? The answers to both questions can be found in Figure 3.7. The two structures are each regular stackings of close-packed planes. The difference lies in the sequence of packing of these layers. The fcc arrangement is such that the fourth close-packed layer lies precisely above the first one. In the hcp structure, the third close-packed layer lies precisely above the first. The fcc stacking is referred to as an *ABCABC . . . sequence,* and the hcp stacking is referred to as an *ABAB . . . sequence*. This subtle difference can lead to significant differences in material properties, as we shall see in Section 6.3. Typical metals with the hcp structure include Be, Mg, α-Ti, Zn, and Zr.

Although the majority of elemental metals fall within one of the three structural groups just discussed, several display less common structures. We shall not dwell on these cases, which can be found from a careful inspection of Appendix 1.

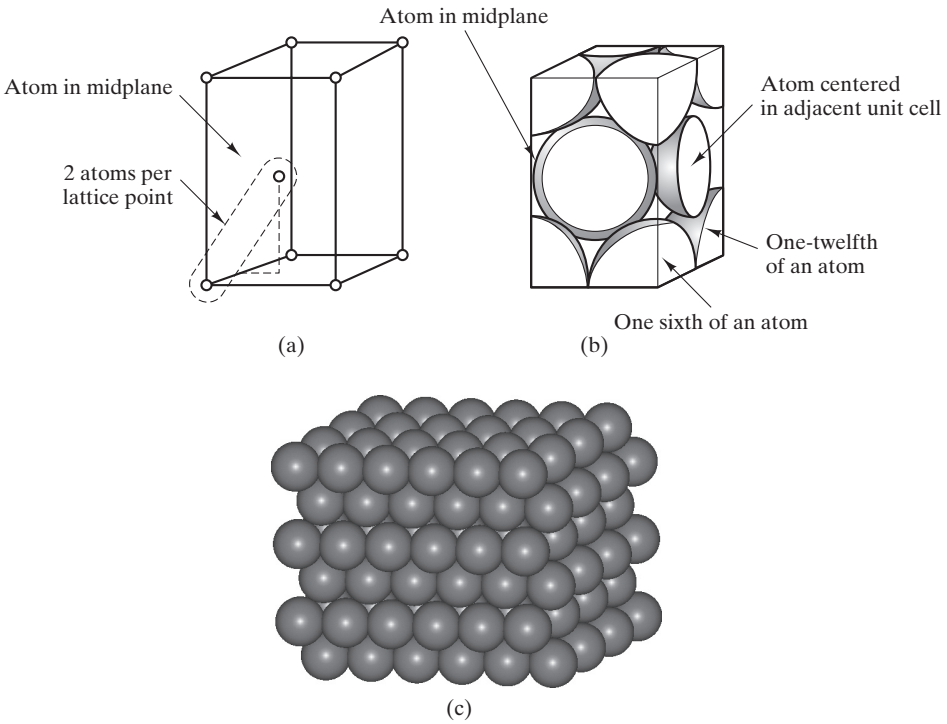


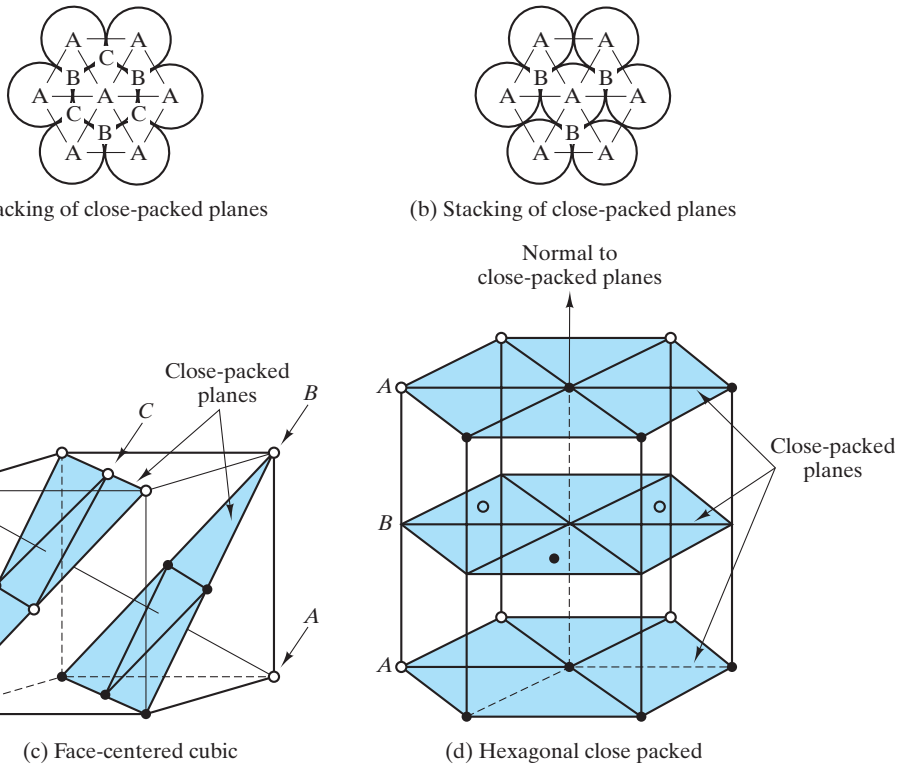
FIGURE 3.6 *Hexagonal close-packed (hcp) structure for metals showing (a) the arrangement of atom centers relative to lattice points for a unit cell. There are two atoms per lattice point (note the outlined example). (b) The actual packing of atoms within the unit cell. Note that the atom in the midplane extends beyond the unit-cell boundaries. (c) The repeating hcp structure, equivalent to many adjacent unit cells. [Part (c) courtesy of Accelrys, Inc.]*

In the course of analyzing the metallic structures introduced in this section, we shall frequently encounter the useful relationships between unit-cell size and atomic radius given in Table 3.3. Our initial discovery of the utility of these relationships is found in the following examples and practice problems.

TABLE 3.3

Relationship between Unit-Cell Size (Edge Length) and Atomic Radius for the Common Metallic Structures

Crystal structure	Relationship between edge length, a, and atomic radius, r
Body-centered cubic (bcc)	$a = 4r/\sqrt{3}$
Face-centered cubic (fcc)	$a = 4r/\sqrt{2}$
Hexagonal close packed (hcp)	$a = 2r$



These atomic scale packing arrangements will appear again in Table 6.8, central to our understanding of the plastic deformation of metals.

FIGURE 3.7 *Comparison of the fcc and hcp structures. They are each efficient stackings of close-packed planes. The difference between the two structures is the different stacking sequences. (From B. D. Cullity and S. R. Stock,* Elements of X-Ray Diffraction*, 3rd ed., Prentice-Hall, Upper Saddle River, NJ, 2001.)*

EXAMPLE 3.2

Using the data of Appendices 1 and 2, calculate the density of copper.

SOLUTION

Appendix 1 shows copper to be an fcc metal. The length, l, of a face diagonal in the unit cell (Figure 3.5) is

$$l = 4r_{\text{Cu atom}} = \sqrt{2}a$$

or

$$a = \frac{4}{\sqrt{2}} r_{\text{Cu atom}},$$

as given in Table 3.3. From the data of Appendix 2,

$$a = \frac{4}{\sqrt{2}}(0.128 \text{ nm}) = 0.362 \text{ nm}.$$