Chapter 3   The Structure of
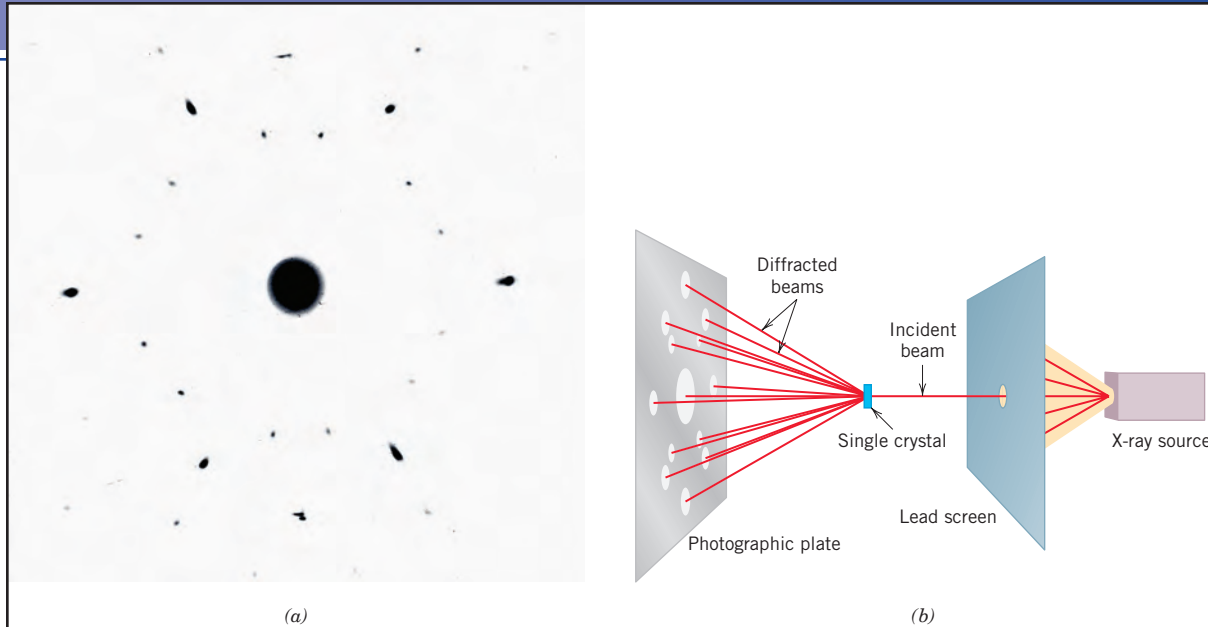   Crystalline Solids

(a)   (b)

(a) X-ray diffraction photograph [or Laue photograph (Section 3.16)] for a single crystal of magnesium. (b) Schematic dia-
gram illustrating how the spots (i.e., the diffraction pattern) in (a) are produced. The lead screen blocks out all beams gener-
ated from the x-ray source, except for a narrow beam traveling in a single direction. This incident beam is diffracted by indi-
vidual crystallographic planes in the single crystal (having different orientations), which gives rise to the various diffracted
beams that impinge on the photographic plate. Intersections of these beams with the plate appear as spots when the film is
developed.

   The large spot in the center of (a) is from the incident beam, which is parallel to a [0001] crystallographic direction. It
should be noted that the hexagonal symmetry of magnesium's hexagonal close-packed crystal structure is indicated by the
diffraction spot pattern that was generated.

   [Figure (a) courtesy of J. G. Byrne, Department of Metallurgical Engineering, University of Utah. Figure (b) from
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WHY STUDY The Structure of Crystalline Solids?

The properties of some materials are directly related
to their crystal structures. For example, pure and un-
deformed magnesium and beryllium, having one crys-
tal structure, are much more brittle (i.e., fracture at
lower degrees of deformation) than are pure and un-
deformed metals such as gold and silver that have yet
another crystal structure (see Section 7.4).

   Furthermore, significant property differences
exist between crystalline and noncrystalline materials
having the same composition. For example, noncrys-
talline ceramics and polymers normally are optically
transparent; the same materials in crystalline (or semi-
crystalline) form tend to be opaque or, at best,
translucent.

Learning Objectives

After studying this chapter you should be able to do the following:

1. Describe the difference in atomic/molecular structure between crystalline and noncrystalline materials.
2. Draw unit cells for face-centered cubic, body-centered cubic, and hexagonal close-packed crystal structures.
3. Derive the relationships between unit cell edge length and atomic radius for face-centered cubic and body-centered cubic crystal structures.
4. Compute the densities for metals having face-centered cubic and body-centered cubic crystal structures given their unit cell dimensions.
5. Given three direction index integers, sketch the direction corresponding to these indices within a unit cell.
6. Specify the Miller indices for a plane that has been drawn within a unit cell.
7. Describe how face-centered cubic and hexagonal close-packed crystal structures may be generated by the stacking of close-packed planes of atoms.
8. Distinguish between single crystals and polycrystalline materials.
9. Define *isotropy* and *anisotropy* with respect to material properties.

3.1 INTRODUCTION

Chapter 2 was concerned primarily with the various types of atomic bonding, which are determined by the electron structures of the individual atoms. The present discussion is devoted to the next level of the structure of materials, specifically, to some of the arrangements that may be assumed by atoms in the solid state. Within this framework, concepts of crystallinity and noncrystallinity are introduced. For crystalline solids the notion of crystal structure is presented, specified in terms of a unit cell. The three common crystal structures found in metals are then detailed, along with the scheme by which crystallographic points, directions, and planes are expressed. Single crystals, polycrystalline, and noncrystalline materials are considered. The final section of this chapter briefly describes how crystal structures are determined experimentally using x-ray diffraction techniques.

Crystal Structures

3.2 FUNDAMENTAL CONCEPTS

crystalline

Solid materials may be classified according to the regularity with which atoms or ions are arranged with respect to one another. A **crystalline** material is one in which the atoms are situated in a repeating or periodic array over large atomic distances; that is, long-range order exists, such that upon solidification, the atoms will position themselves in a repetitive three-dimensional pattern, in which each atom is bonded to its nearest-neighbor atoms. All metals, many ceramic materials, and certain polymers form crystalline structures under normal solidification conditions. For those that do not crystallize, this long-range atomic order is absent; these *noncrystalline* or *amorphous* materials are discussed briefly at the end of this chapter.

crystal structure

Some of the properties of crystalline solids depend on the **crystal structure** of the material, the manner in which atoms, ions, or molecules are spatially arranged. There is an extremely large number of different crystal structures all having long-range atomic order; these vary from relatively simple structures for metals to exceedingly complex ones, as displayed by some of the ceramic and polymeric materials. The present discussion deals with several common metallic crystal structures. Chapters 12 and 14 are devoted to crystal structures for ceramics and polymers, respectively.
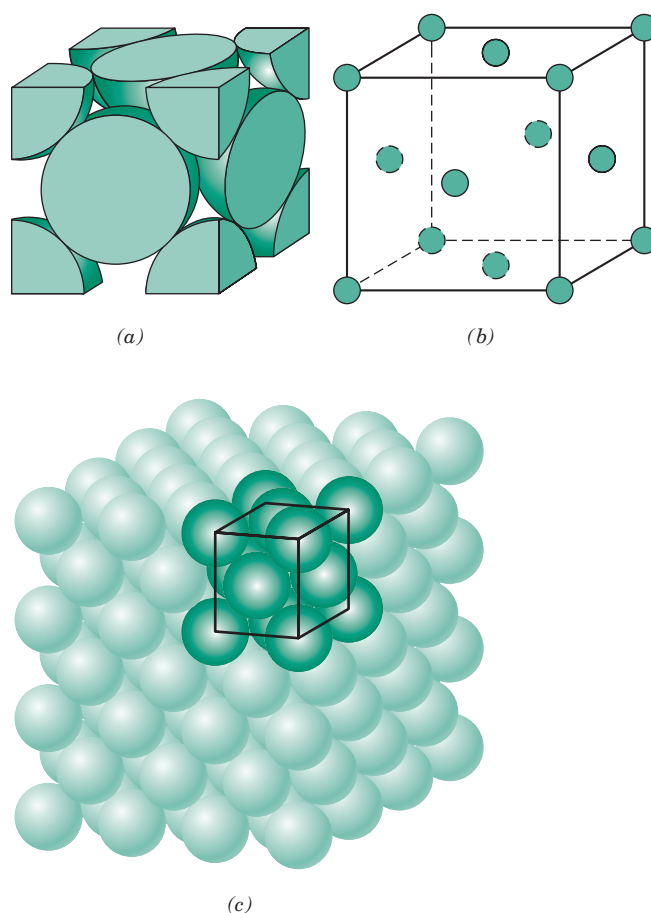
(a)

(b)

Figure 3.1 For the face-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*) adapted 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.]

(c)

When describing crystalline structures, atoms (or ions) are thought of as being solid spheres having well-defined diameters. This is termed the *atomic hard sphere model* in which spheres representing nearest-neighbor atoms touch one another. An example of the hard sphere model for the atomic arrangement found in some of the common elemental metals is displayed in Figure 3.1*c*. In this particular case all the atoms are identical. Sometimes the term **lattice** is used in the context of crystal structures; in this sense "lattice" means a three-dimensional array of points coinciding with atom positions (or sphere centers).

lattice

3.3 UNIT CELLS

unit cell

The atomic order in crystalline solids indicates that small groups of atoms form a repetitive pattern. Thus, in describing crystal structures, it is often convenient to subdivide the structure into small repeat entities called **unit cells.** Unit cells for most crystal structures are parallelepipeds or prisms having three sets of parallel faces; one is drawn within the aggregate of spheres (Figure 3.1*c*), which in this case happens to be a cube. A unit cell is chosen to represent the symmetry of the crystal structure, wherein all the atom positions in the crystal may be generated by translations of the unit cell integral distances along each of its edges. Thus, the unit cell is the basic structural unit or building block of the crystal structure and defines the crystal structure by virtue of its geometry and the atom positions within.