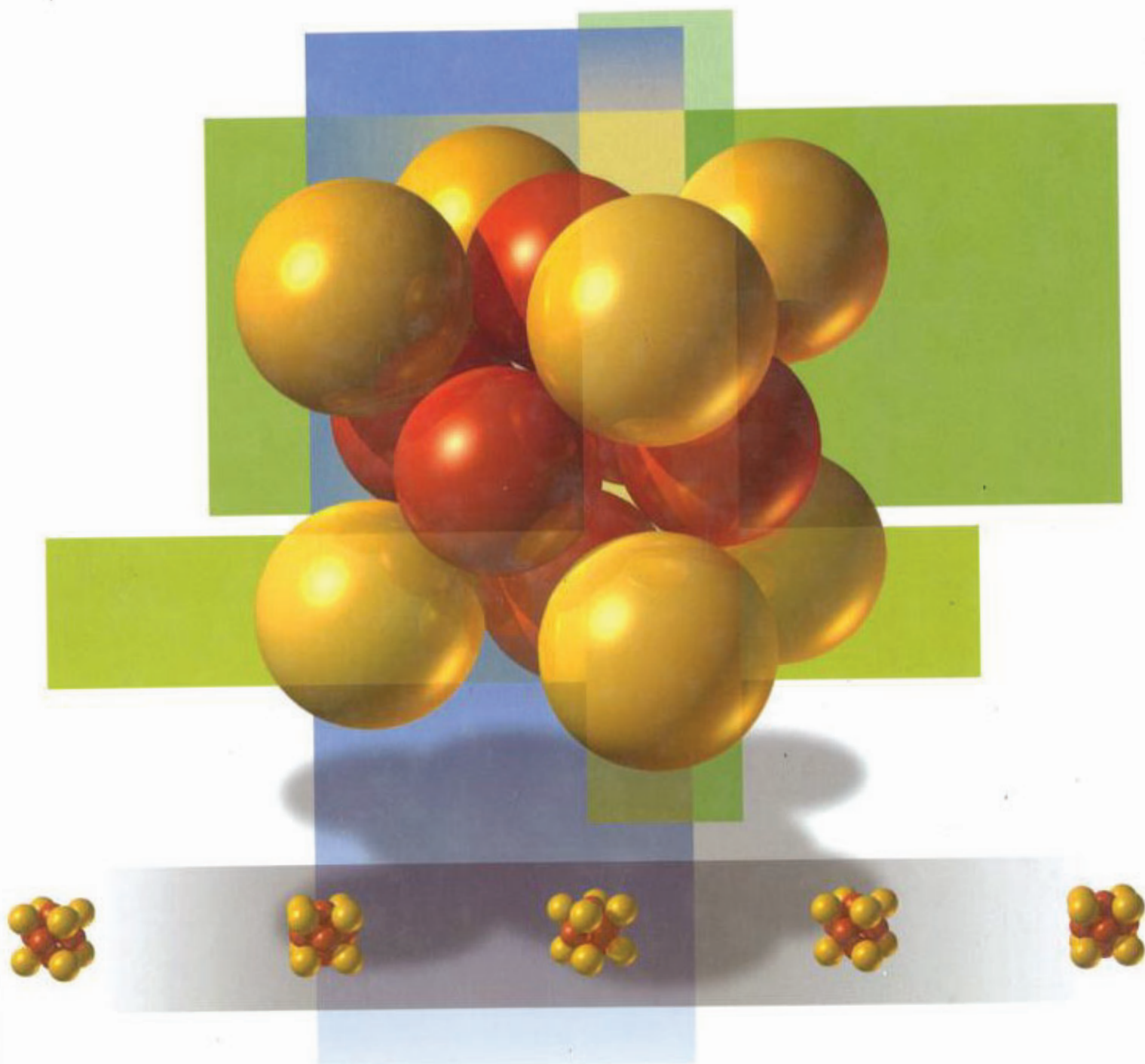


FUNDAMENTALS OF

# Materials Science and Engineering

| An Integrated Approach

Second Edition



William D. Callister, Jr.

IP Bridge Exhibit 2009  
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SECOND EDITION

# Fundamentals of Materials Science and Engineering

## An Integrated Approach

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**John Wiley & Sons, Inc.**

**Front Cover:** The object that appears on the front cover represents a unit cell for the intermetallic compound  $\text{AuCu}_3$ . The yellow and brown spheres represent gold and copper atoms, respectively.

**Back Cover:** Depiction of a unit cell for the intermetallic compound  $\text{AuCu}$ . Again, the yellow and brown spheres represent gold and copper atoms.

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each of the eight corner atoms and one half of each of the six face atoms, or a total of four whole atoms, may be assigned to a given unit cell. This is depicted in Figure 3.1a, where only sphere portions are represented within the confines of the cube. The cell comprises the volume of the cube, which is generated from the centers of the corner atoms as shown in the figure.

Corner and face positions are really equivalent; that is, translation of the cube corner from an original corner atom to the center of a face atom will not alter the cell structure.

Two other important characteristics of a crystal structure are the **coordination number** and the **atomic packing factor (APF)**. 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

$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}} \quad (3.2)$$

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. Metals typically have relatively large atomic packing factors to maximize the shielding provided by the free electron cloud.



### 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 of BCC unit cells with the atoms represented by hard sphere and reduced-sphere

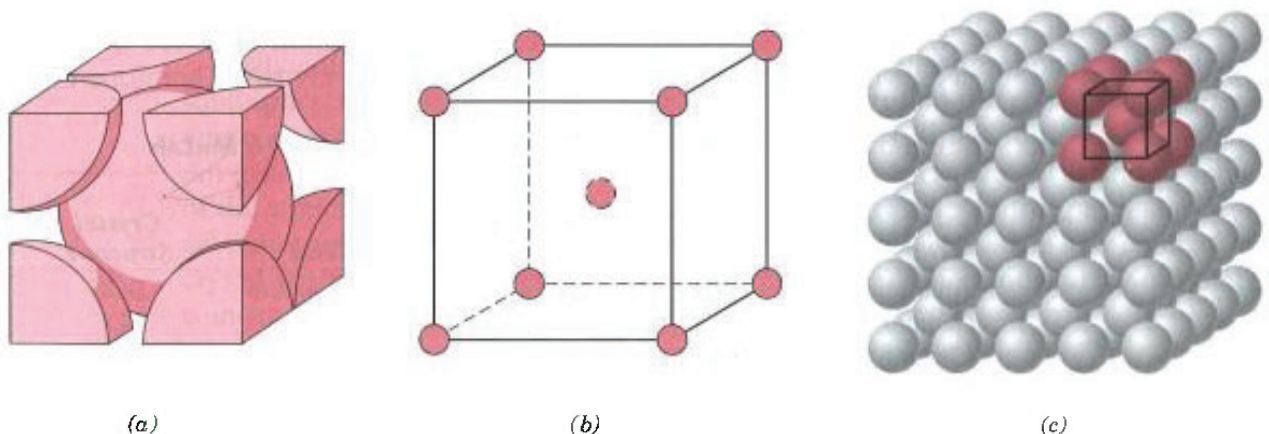


**Figure 3.2** For the body-centered cubic crystal structure, (a) a hard sphere unit cell representation, (b) a reduced-sphere unit cell, and (c) an aggregate of many atoms. (Figure (c) from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. I, *Structure*,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

models, respectively. Center and corner atoms touch one another along cube diagonals, and unit cell length  $a$  and atomic radius  $R$  are related through

$$a = \frac{4R}{\sqrt{3}} \quad (3.3)$$

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

Two atoms are associated with each BCC unit cell: the equivalent of one atom from the eight corners, each of which is shared among eight unit cells, and the single center atom, which is wholly contained within its cell. In addition, corner and center atom positions are equivalent. 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.



### 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.<sup>1</sup> 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

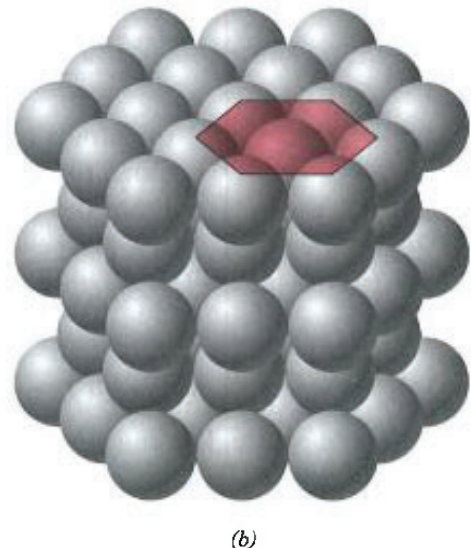
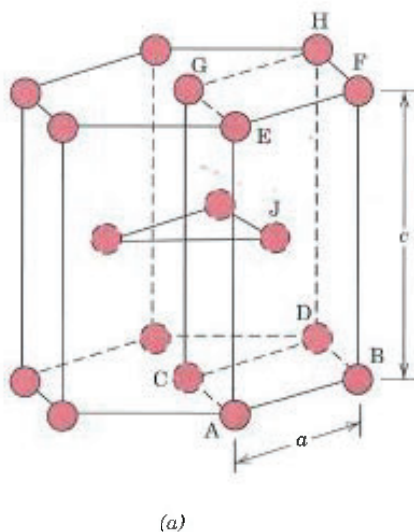


**Figure 3.3** For the hexagonal close-packed crystal structure, (a) a reduced-sphere unit cell ( $a$  and  $c$  represent the short and long edge lengths, respectively), and (b) an aggregate of many atoms. (Figure (b) from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of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

<sup>1</sup> Alternatively, the unit cell for HCP may be specified in terms of the parallelepiped defined by atoms labeled A through H in Figure 3.3. As such, the atom denoted J lies within the unit cell interior.

# Glossary

## A

**Abrasive.** A hard and wear-resistant material (commonly a ceramic) that is used to wear, grind, or cut away other material.

**Absorption.** The optical phenomenon whereby the energy of a photon of light is assimilated within a substance, normally by electronic polarization or by an electron excitation event.

**Acceptor level.** For a semiconductor or insulator, an energy level lying within yet near the bottom of the energy band gap, which may accept electrons from the valence band, leaving behind holes. The level is normally introduced by an impurity atom.

**Activation energy ( $Q$ ).** The energy required to initiate a reaction, such as diffusion.

**Activation polarization.** The condition wherein the rate of an electrochemical reaction is controlled by the one slowest step in a sequence of steps that occur in series.

**Addition (or chain reaction) polymerization.** The process by which bifunctional monomer units are attached one at a time, in chainlike fashion, to form a linear polymer macromolecule.

**Adhesive.** A substance that bonds together the surfaces of two other materials (termed adherends).

**Age hardening.** See **Precipitation hardening**.

**Allotropy.** The possibility of existence of two or more different crystal structures for a substance (generally an elemental solid).

**Alloy.** A metallic substance that is composed of two or more elements.

**Alloy steel.** A ferrous (or iron-based) alloy that contains appreciable concentrations of alloying elements (other than C and residual amounts of Mn, Si, S, and P). These alloying elements are usually added to improve mechanical and corrosion resistance properties.

**Alternating copolymer.** A copolymer in which two different mer units alternate positions along the molecular chain.

**Amorphous.** Having a noncrystalline structure.

**Anelastic deformation.** Time-dependent elastic (nonpermanent) deformation.

**Anion.** A negatively charged, non-metallic ion.

**Anisotropic.** Exhibiting different values of a property in different crystallographic directions.

**Annealing.** A generic term used to denote a heat treatment wherein the microstructure and, consequently, the properties of a material are altered. "Annealing" frequently refers to a heat treatment whereby a previously cold-worked metal is softened by allowing it to recrystallize.

**Annealing point (glass).** That temperature at which residual stresses in a glass are eliminated within about 15 min; this corresponds to a glass viscosity of about  $10^{12}$  Pa-s ( $10^{13}$  P).

**Anode.** The electrode in an electrochemical cell or galvanic couple that experiences oxidation, or gives up electrons.

**Antiferromagnetism.** A phenomenon observed in some materials (e.g., MnO); complete magnetic

moment cancellation occurs as a result of antiparallel coupling of adjacent atoms or ions. The macroscopic solid possesses no net magnetic moment.

**Artificial aging.** For precipitation hardening, aging above room temperature.

**Atactic.** A type of polymer chain configuration wherein side groups are randomly positioned on one side of the chain or the other.

**Athermal transformation.** A reaction that is not thermally activated, and usually diffusionless, as with the martensitic transformation. Normally, the transformation takes place with great speed (i.e., is independent of time), and the extent of reaction depends on temperature.

**Atomic mass unit (amu).** A measure of atomic mass; one twelfth of the mass of an atom of  $C^{12}$ .

**Atomic number ( $Z$ ).** For a chemical element, the number of protons within the atomic nucleus.

**Atomic packing factor (APF).** The fraction of the volume of a unit cell that is occupied by "hard sphere" atoms or ions.

**Atomic vibration.** The vibration of an atom about its normal position in a substance.

**Atomic weight ( $A$ ).** The weighted average of the atomic masses of an atom's naturally occurring isotopes. It may be expressed in terms of atomic mass units (on an atomic basis), or the mass per mole of atoms.

**Atom percent (at%).** Concentration specification on the basis of the number of moles (or atoms) of a particular element relative to the