EXAMPLE PROBLEM 4.1

Number-of-Vacancies Computation at a Specified Temperature

Calculate the equilibrium number of vacancies per cubic meter for copper at 1000°C. The energy for vacancy formation is 0.9 eV/atom; the atomic weight and density (at 1000°C) for copper are 63.5 g/mol and 8.4 g/cm³, respectively.

Solution

This problem may be solved by using Equation 4.1; it is first necessary, however, to determine the value of N—the number of atomic sites per cubic meter for copper, from its atomic weight A_{Cu}, its density ρ, and Avogadro's number N_A, according to

Number of atoms per unit volume for a metal

$$N = \frac{N_A \rho}{A_{Cu}} \qquad (4.2)$$

$$= \frac{(6.022 \times 10^{23} \text{ atoms/mol})(8.4 \text{ g/cm}^3)(10^6 \text{ cm}^3/\text{m}^3)}{63.5 \text{ g/mol}}$$

$$= 8.0 \times 10^{28} \text{ atoms/m}^3$$

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Thus, the number of vacancies at 1000°C (1273 K) is equal to

$$N_v = N \exp\left(-\frac{Q_v}{kT}\right)$$

$$= (8.0 \times 10^{28} \text{ atoms/m}^3) \exp\left[-\frac{(0.9 \text{ eV})}{(8.62 \times 10^{-5} \text{ eV/K})(1273 \text{ K})}\right]$$

$$= 2.2 \times 10^{25} \text{ vacancies/m}^3$$

4.3 IMPURITIES IN SOLIDS

A pure metal consisting of only one type of atom just isn't possible; impurity or foreign atoms are always present, and some exist as crystalline point defects. In fact, even with relatively sophisticated techniques, it is difficult to refine metals to a purity in excess of 99.9999%. At this level, on the order of 10^{22} to 10^{23} impurity atoms are present in

alloy

1 m³ of material. Most familiar metals are not highly pure; rather, they are **alloys,** in which impurity atoms have been added intentionally to impart specific characteristics to the material. Ordinarily, alloying is used in metals to improve mechanical strength and corrosion resistance. For example, sterling silver is a 92.5% silver/7.5% copper alloy. In normal ambient environments, pure silver is highly corrosion resistant, but also very soft. Alloying with copper significantly enhances the mechanical strength without depreciating the corrosion resistance appreciably.

solid solution

The addition of impurity atoms to a metal results in the formation of a **solid solution** and/or a new *second phase,* depending on the kinds of impurity, their concentrations, and the temperature of the alloy. The present discussion is concerned with the notion of a solid solution; treatment of the formation of a new phase is deferred to Chapter 9.

Several terms relating to impurities and solid solutions deserve mention. With re-

solute, solvent

gard to alloys, **solute** and **solvent** are terms that are commonly employed. *Solvent* is the element or compound that is present in the greatest amount; on occasion, solvent atoms are also called *host atoms*. *Solute* is used to denote an element or compound present in a minor concentration.

Figure 4.3
Locations of tetrahedral and octahedral interstitial sites within (*a*) FCC and (*b*) BCC unit cells.
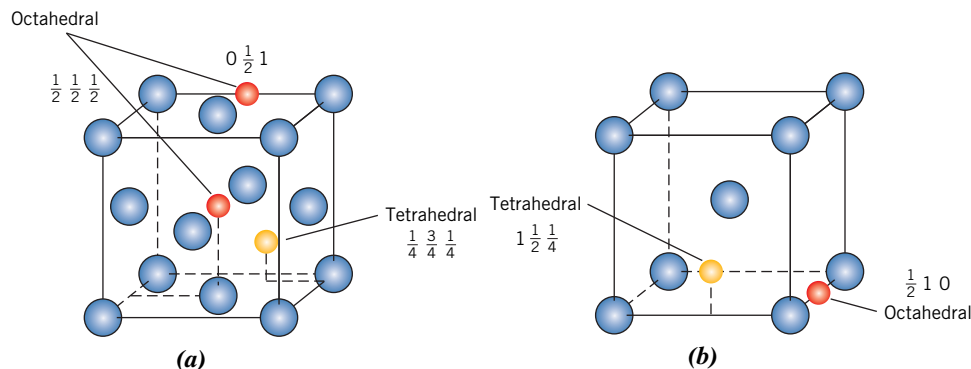
sites have a coordination number of 4; straight lines drawn from the centers of the surrounding host atoms form a four-sided tetrahedron. However, for octahedral sites the coordination number is 6; an octahedron is produced by joining these six sphere centers.[3] For FCC, there are two types of octahedral sites with representative point coordinates of $0\frac{1}{2}1$ and $\frac{1}{2}\frac{1}{2}\frac{1}{2}$. Representative coordinates for a single tetrahedral site type are $\frac{1}{4}\frac{3}{4}\frac{1}{4}$.[4] Locations of these sites within the FCC unit cell are noted in Figure 4.3*a*. One type of each of octahedral and tetrahedral interstitial sites is found for BCC. Representative coordinates are as follows: octahedral, $\frac{1}{2}10$ and tetrahedral, $1\frac{1}{2}\frac{1}{4}$. Figure 4.3*b* shows the positions of these sites within a BCC unit cell.[4]

Metallic materials have relatively high atomic packing factors, which means that these interstitial positions are relatively small. Consequently, the atomic diameter of an interstitial impurity must be substantially smaller than that of the host atoms. Normally, the maximum allowable concentration of interstitial impurity atoms is low (less than 10%). Even very small impurity atoms are ordinarily larger than the interstitial sites, and as a consequence, they introduce some lattice strains on the adjacent host atoms. Problems 4.8 and 4.9 call for determination of the radii of impurity atoms *r* (in terms of *R*, the host atom radius) that just fit into tetrahedral and octahedral interstitial positions of both BCC and FCC without introducing any lattice strains.

Carbon forms an interstitial solid solution when added to iron; the maximum concentration of carbon is about 2%. The atomic radius of the carbon atom is much less than that of iron: 0.071 nm versus 0.124 nm.

Solid solutions are also possible for ceramic materials, as discussed in Section 12.5.

EXAMPLE PROBLEM 4.2

Computation of Radius of BCC Interstitial Site

Compute the radius *r* of an impurity atom that just fits into a BCC octahedral site in terms of the atomic radius *R* of the host atom (without introducing lattice strains).

Solution

As Figure 4.3*b* notes, for BCC, the octahedral interstitial site is situated at the center of a unit cell edge. In order for an interstitial atom to be positioned in this site without introducing lattice

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[3]The geometries of these site types may be observed in Figure 12.7.

[4]Other octahedral and tetrahedral interstices are located at positions within the unit cell that are equivalent to these representative ones.

strains, the atom just touches the two adjacent host atoms, which are corner atoms of the unit cell. The drawing shows atoms on the (100) face of a BCC unit cell; the large circles represent the host atoms—the small circle represents an interstitial atom that is positioned in an octahedral site on the cube edge.

On this drawing is noted the unit cell edge length—the distance between the centers of the corner atoms—which, from Equation 3.4, is equal to

$$\text{Unit cell edge length} = \frac{4R}{\sqrt{3}}$$

Also shown is that the unit cell edge length is equal to two times the sum of host atomic radius $2R$ plus twice the radius of the interstitial atom $2r$; i.e.,

$$\text{Unit cell edge length} = 2R + 2r$$

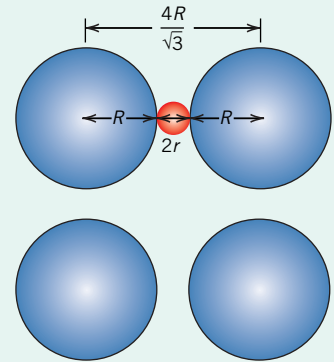Now, equating these two unit cell edge length expressions, we get

$$2R + 2r = \frac{4R}{\sqrt{3}}$$

and solving for r in terms of R

$$2r = \frac{4R}{\sqrt{3}} - 2R = \left(\frac{2}{\sqrt{3}} - 1\right)(2R)$$

or

$$r = \left(\frac{2}{\sqrt{3}} - 1\right)R = 0.155R$$

✓ **Concept Check 4.1**   Is it possible for three or more elements to form a solid solution? Explain your answer.

[*The answer may be found at www.wiley.com/college/callister (Student Companion Site)*].

✓ **Concept Check 4.2**   Explain why complete solid solubility may occur for substitutional solid solutions but not for interstitial solid solutions.

[*The answer may be found at www.wiley.com/college/callister (Student Companion Site)*].

4.4 SPECIFICATION OF COMPOSITION

composition

weight percent

It is often necessary to express the **composition** (or *concentration*)[5] of an alloy in terms of its constituent elements. The two most common ways to specify composition are weight (or mass) percent and atom percent. The basis for **weight percent** (wt%) is the weight of a particular element relative to the total alloy weight. For an alloy that

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[5]The terms *composition* and *concentration* will be assumed to have the same meaning in this book (i.e., the relative content of a specific element or constituent in an alloy) and will be used interchangeably.

reasonably valid assumption and does not lead to significant errors for dilute solutions and over composition ranges where solid solutions exist.

EXAMPLE PROBLEM 4.3

Derivation of Composition-Conversion Equation

Derive Equation 4.6a.

Solution

To simplify this derivation, we assume that masses are expressed in units of grams and denoted with a prime (e.g., m_1'). Furthermore, the total alloy mass (in grams) M' is

$$M' = m_1' + m_2' \tag{4.12}$$

Using the definition of C_1' (Equation 4.5a) and incorporating the expression for n_{m1}, Equation 4.4, and the analogous expression for n_{m2} yields

$$C_1' = \frac{n_{m1}}{n_{m1} + n_{m2}} \times 100$$

$$= \frac{\dfrac{m_1'}{A_1}}{\dfrac{m_1'}{A_1} + \dfrac{m_2'}{A_2}} \times 100 \tag{4.13}$$

Rearrangement of the mass-in-grams equivalent of Equation 4.3a leads to

$$m_1' = \frac{C_1 M'}{100} \tag{4.14}$$

Substitution of this expression and its m_2' equivalent into Equation 4.13 gives

$$C_1' = \frac{\dfrac{C_1 M'}{100 A_1}}{\dfrac{C_1 M'}{100 A_1} + \dfrac{C_2 M'}{100 A_2}} \times 100 \tag{4.15}$$

Upon simplification, we have

$$C_1' = \frac{C_1 A_2}{C_1 A_2 + C_2 A_1} \times 100$$

which is identical to Equation 4.6a.

EXAMPLE PROBLEM 4.4

Composition Conversion—From Weight Percent to Atom Percent

Determine the composition, in atom percent, of an alloy that consists of 97 wt% aluminum and 3 wt% copper.

Solution

If we denote the respective weight percent compositions as $C_{Al} = 97$ and $C_{Cu} = 3$, substitution into Equations 4.6a and 4.6b yields

and

$$C'_{Al} = \frac{C_{Al}A_{Cu}}{C_{Al}A_{Cu} + C_{Cu}A_{Al}} \times 100$$

$$= \frac{(97)(63.55 \text{ g/mol})}{(97)(63.55 \text{ g/mol}) + (3)(26.98 \text{ g/mol})} \times 100$$

$$= 98.7 \text{ at\%}$$

$$C'_{Cu} = \frac{C_{Cu}A_{Al}}{C_{Cu}A_{Al} + C_{Al}A_{Cu}} \times 100$$

$$= \frac{(3)(26.98 \text{ g/mol})}{(3)(26.98 \text{ g/mol}) + (97)(63.55 \text{ g/mol})} \times 100$$

$$= 1.30 \text{ at\%}$$

Miscellaneous Imperfections

4.5 DISLOCATIONS—LINEAR DEFECTS

edge dislocation

dislocation line

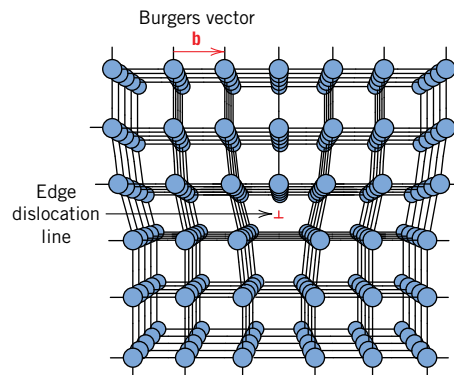**screw dislocation**

A *dislocation* is a linear or one-dimensional defect around which some of the atoms are misaligned. One type of dislocation is represented in Figure 4.4: an extra portion of a plane of atoms, or half-plane, the edge of which terminates within the crystal. This is termed an **edge dislocation;** it is a linear defect that centers on the line that is defined along the end of the extra half-plane of atoms. This is sometimes termed the **dislocation line,** which, for the edge dislocation in Figure 4.4, is perpendicular to the plane of the page. Within the region around the dislocation line there is some localized lattice distortion. The atoms above the dislocation line in Figure 4.4 are squeezed together, and those below are pulled apart; this is reflected in the slight curvature for the vertical planes of atoms as they bend around this extra half-plane. The magnitude of this distortion decreases with distance away from the dislocation line; at positions far removed, the crystal lattice is virtually perfect. Sometimes the edge dislocation in Figure 4.4 is represented by the symbol ⊥, which also indicates the position of the dislocation line. An edge dislocation may also be formed by an extra half-plane of atoms that is included in the bottom portion of the crystal; its designation is a ⊤.

Another type of dislocation, called a **screw dislocation,** may be thought of as being formed by a shear stress that is applied to produce the distortion shown in Figure 4.5*a:* the

Figure 4.4 The atom positions around an edge dislocation; extra half-plane of atoms shown in perspective.
(Adapted from A. G. Guy, *Essentials of Materials Science,* McGraw-Hill Book Company, New York, NY, 1976, p. 153.)

Burgers vector
b

Edge
dislocation
line