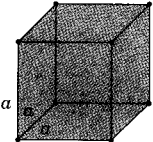
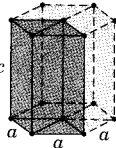
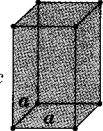
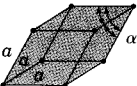
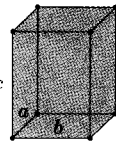
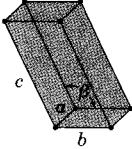
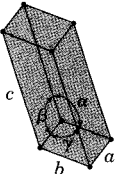


Table 3.2 Lattice Parameter Relationships and Figures Showing Unit Cell Geometries for the Seven Crystal Systems

<i>Crystal System</i>	<i>Axial Relationships</i>	<i>Interaxial Angles</i>	<i>Unit Cell Geometry</i>
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	
Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$	
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90^\circ \neq \beta$	
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	

most often described in terms of unit cells, which are normally more complex than those for FCC, BCC, and HCP. In addition, for these other systems, we are often interested in determining atomic packing factors and densities, using modified forms of Equations 3.2 and 3.5. Furthermore, according to unit cell geometry, crystal structures of these other material types are grouped within the seven crystal systems.

CRYSTALLOGRAPHIC DIRECTIONS AND PLANES

When dealing with crystalline materials, it often becomes necessary to specify some particular crystallographic plane of atoms or a crystallographic direction. Labeling conventions have been established in which three integers or indices are used to designate directions and planes. The basis for determining index values is the unit cell, with a coordinate system consisting of three (x , y , and z) axes situated at one of the corners and coinciding with the unit cell edges, as shown in Figure 3.4. For some crystal systems—namely, hexagonal, rhombohedral, monoclinic, and triclinic—the three axes are *not* mutually perpendicular, as in the familiar Cartesian coordinate scheme.

3.8 CRYSTALLOGRAPHIC DIRECTIONS



A crystallographic direction is defined as a line between two points, or a vector. The following steps are utilized in the determination of the three directional indices:

1. A vector of convenient length is positioned such that it passes through the origin of the coordinate system. Any vector may be translated throughout the crystal lattice without alteration, if parallelism is maintained.
2. The length of the vector projection on each of the three axes is determined; *these are measured in terms of the unit cell dimensions a , b , and c .*
3. These three numbers are multiplied or divided by a common factor to reduce them to the smallest integer values.
4. The three indices, not separated by commas, are enclosed in square brackets, thus: $[uvw]$. The u , v , and w integers correspond to the reduced projections along the x , y , and z axes, respectively.

For each of the three axes, there will exist both positive and negative coordinates. Thus negative indices are also possible, which are represented by a bar over the appropriate index. For example, the $[\bar{1}\bar{1}\bar{1}]$ direction would have a component in the $-y$ direction. Also, changing the signs of all indices produces an antiparallel direction; that is, $[\bar{1}\bar{1}\bar{1}]$ is directly opposite to $[1\bar{1}\bar{1}]$. If more than one direction or plane is to be specified for a particular crystal structure, it is imperative for the maintaining of consistency that a positive–negative convention, once established, not be changed.

The $[100]$, $[110]$, and $[111]$ directions are common ones; they are drawn in the unit cell shown in Figure 3.5.

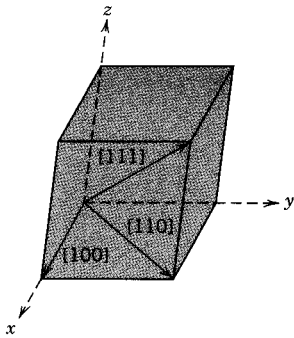
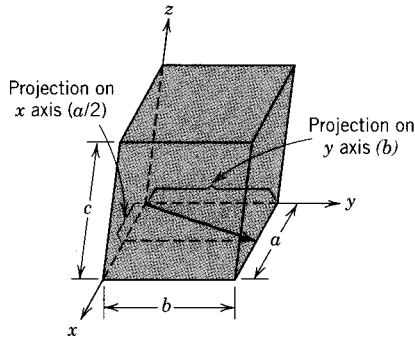


FIGURE 3.5 The [100], [110], and [111] directions within a unit cell.

EXAMPLE PROBLEM 3.4

Determine the indices for the direction shown in the accompanying figure.



SOLUTION

The vector, as drawn, passes through the origin of the coordinate system, and therefore no translation is necessary. Projections of this vector onto the x , y , and z axes are, respectively, $a/2$, b , and $0c$, which become $\frac{1}{2}$, 1 , and 0 in terms of the unit cell parameters (i.e., when the a , b , and c are dropped). Reduction of these numbers to the lowest set of integers is accompanied by multiplication of each by the factor 2. This yields the integers 1, 2, and 0, which are then enclosed in brackets as [120].

This procedure may be summarized as follows:

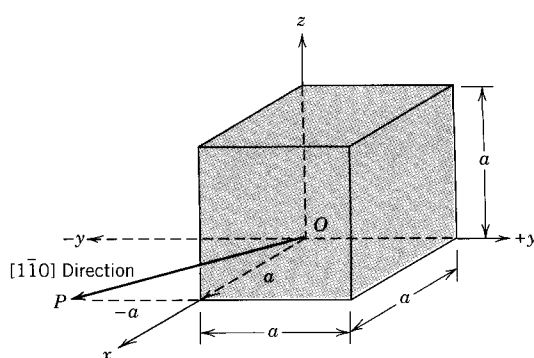
	x	y	z
Projections	$a/2$	b	$0c$
Projections (in terms of a , b , and c)	$\frac{1}{2}$	1	0
Reduction	1	2	0
Enclosure	[120]		

EXAMPLE PROBLEM 3.5

Draw a $[\bar{1}10]$ direction within a cubic unit cell.

SOLUTION

First construct an appropriate unit cell and coordinate axes system. In the accompanying figure the unit cell is cubic, and the origin of the coordinate system, point O , is located at one of the cube corners.



This problem is solved by reversing the procedure of the preceding example. For this $[1\bar{1}0]$ direction, the projections along the x , y , z axes are a , $-a$, and $0a$, respectively. This direction is defined by a vector passing from the origin to point P , which is located by first moving along the x axis a units, and from this position, parallel to the y axis $-a$ units, as indicated in the figure. There is no z component to the vector, since the z projection is zero.

For some crystal structures, several nonparallel directions with different indices are actually equivalent; this means that the spacing of atoms along each direction is the same. For example, in cubic crystals, all the directions represented by the following indices are equivalent: $[100]$, $[\bar{1}00]$, $[010]$, $[0\bar{1}0]$, $[001]$, and $[00\bar{1}]$. As a convenience, equivalent directions are grouped together into a *family*, which are enclosed in angle brackets, thus: $\langle 100 \rangle$. Furthermore, directions in cubic crystals having the same indices without regard to order or sign, for example, $[123]$ and $[\bar{2}\bar{1}\bar{3}]$, are equivalent. This is, in general, not true for other crystal systems. For example, for crystals of tetragonal symmetry, $[100]$ and $[010]$ directions are equivalent, whereas $[100]$ and $[001]$ are not.

HEXAGONAL CRYSTALS

A problem arises for crystals having hexagonal symmetry in that some crystallographic equivalent directions will not have the same set of indices. This is circumvented by utilizing a four-axis, or *Miller-Bravais*, coordinate system as shown in Figure 3.6. The three a_1 , a_2 , and a_3 axes are all contained within a single plane (called the basal plane), and at 120° angles to one another. The z axis is perpendicular

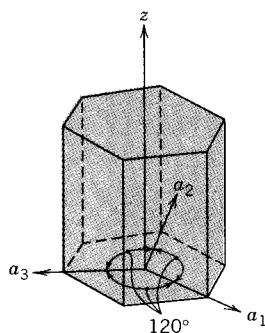


FIGURE 3.6 Coordinate axis system for a hexagonal unit cell (Miller-Bravais scheme).

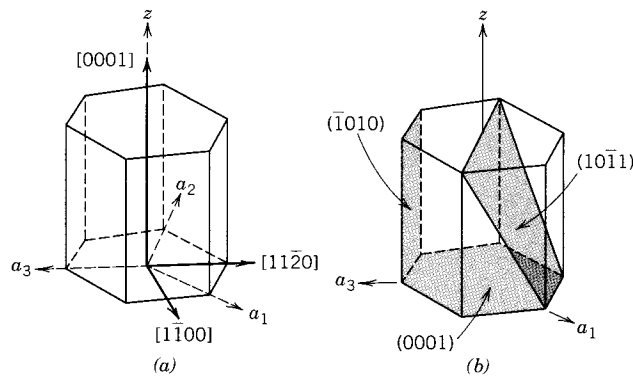


FIGURE 3.7 For the hexagonal crystal system, (a) $[0001]$, $[1\bar{1}00]$, and $[11\bar{2}0]$ directions, and (b) the (0001) , $(10\bar{1}1)$, and $(\bar{1}010)$ planes.

to this basal plane. Directional indices, which are obtained as described above, will be denoted by four indices, as $[uvw]$; by convention, the first three indices pertain to projections along the respective a_1 , a_2 , and a_3 axes in the basal plane.

Conversion from the three-index system to the four-index system,

$$[u'v'w'] \longrightarrow [uvw]$$

is accomplished by the following formulas:

$$u = \frac{n}{3}(2u' - v') \quad (3.6a)$$

$$v = \frac{n}{3}(2v' - u') \quad (3.6b)$$

$$t = -(u + v) \quad (3.6c)$$

$$w = nw' \quad (3.6d)$$

where primed indices are associated with the three-index scheme and unprimed, with the new Miller–Bravais four-index system; n is a factor that may be required to reduce u , v , t , and w to the smallest integers. For example, using this conversion, the $[010]$ direction becomes $[\bar{1}2\bar{1}0]$. Several different directions are indicated in the hexagonal unit cell (Figure 3.7a).

3.9 CRYSTALLOGRAPHIC PLANES



The orientations of planes for a crystal structure are represented in a similar manner. Again, the unit cell is the basis, with the three-axis coordinate system as represented in Figure 3.4. In all but the hexagonal crystal system, crystallographic planes are specified by three **Miller indices** as (hkl) . Any two planes parallel to each other are equivalent and have identical indices. The procedure employed in determination of the h , k , and l index numbers is as follows:

1. If the plane passes through the selected origin, either another parallel plane must be constructed within the unit cell by an appropriate translation, or a new origin must be established at the corner of another unit cell.
2. At this point the crystallographic plane either intersects or parallels each of the three axes; the length of the planar intercept for each axis is determined in terms of the lattice parameters a , b , and c .

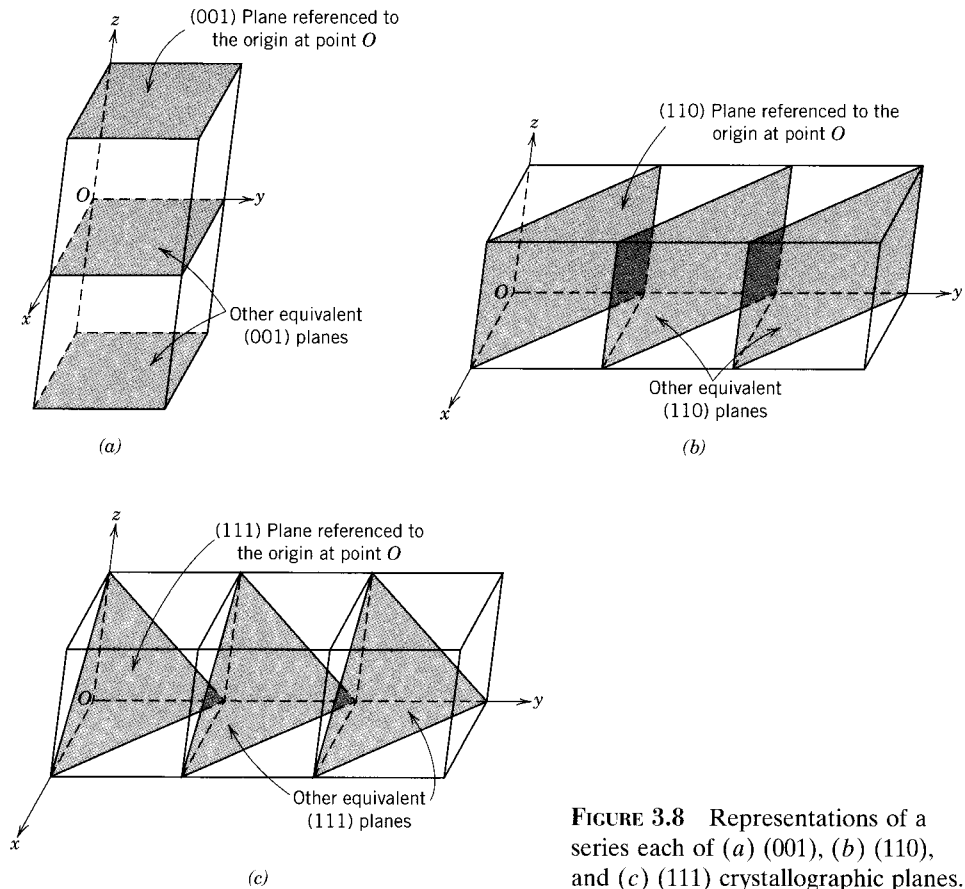


FIGURE 3.8 Representations of a series each of (a) (001), (b) (110), and (c) (111) crystallographic planes.

3. The reciprocals of these numbers are taken. A plane that parallels an axis may be considered to have an infinite intercept, and, therefore, a zero index.
4. If necessary, these three numbers are changed to the set of smallest integers by multiplication or division by a common factor.¹
5. Finally, the integer indices, not separated by commas, are enclosed within parentheses, thus: (hkl) .

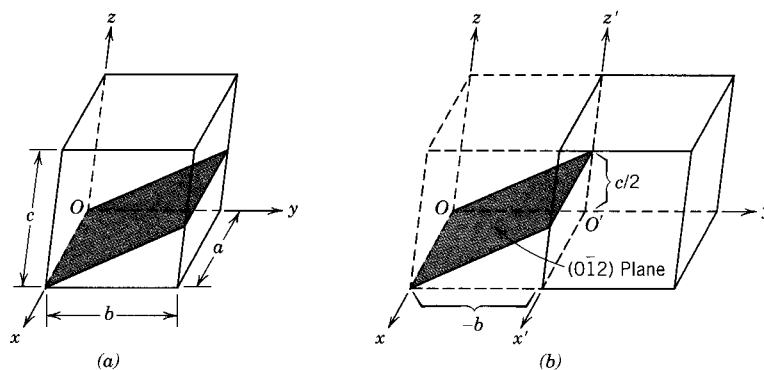
An intercept on the negative side of the origin is indicated by a bar or minus sign positioned over the appropriate index. Furthermore, reversing the directions of all indices specifies another plane parallel to, on the opposite side of and equidistant from, the origin. Several low-index planes are represented in Figure 3.8.

One interesting and unique characteristic of cubic crystals is that planes and directions having the same indices are perpendicular to one another; however, for other crystal systems there are no simple geometrical relationships between planes and directions having the same indices.

¹ On occasion, index reduction is not carried out (e.g., for x-ray diffraction studies that are described in Section 3.15); for example, (002) is not reduced to (001). In addition, for ceramic materials, the ionic arrangement for a reduced-index plane may be different from that for a nonreduced one.

EXAMPLE PROBLEM 3.6

Determine the Miller indices for the plane shown in the accompanying sketch (a).

**SOLUTION**

Since the plane passes through the selected origin O , a new origin must be chosen at the corner of an adjacent unit cell, taken as O' and shown in sketch (b). This plane is parallel to the x axis, and the intercept may be taken as ∞a . The y and z axes intersections, referenced to the new origin O' , are $-b$ and $c/2$, respectively. Thus, in terms of the lattice parameters a , b , and c , these intersections are ∞ , -1 , and $\frac{1}{2}$. The reciprocals of these numbers are 0 , -1 , and 2 ; and since all are integers, no further reduction is necessary. Finally, enclosure in parentheses yields $(0\bar{1}2)$.

These steps are briefly summarized below:

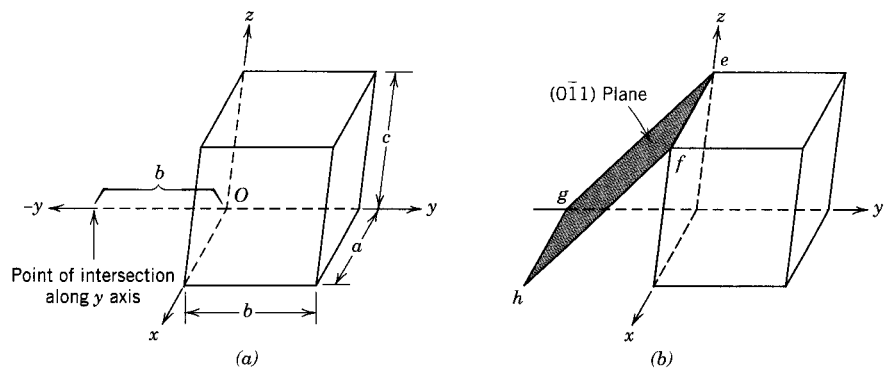
	x	y	z
Intercepts	∞a	$-b$	$c/2$
Intercepts (in terms of lattice parameters)	∞	-1	$\frac{1}{2}$
Reciprocals	0	-1	2
Reductions (unnecessary)			
Enclosure		$(0\bar{1}2)$	

EXAMPLE PROBLEM 3.7

Construct a $(0\bar{1}1)$ plane within a cubic unit cell.

SOLUTION

To solve this problem, carry out the procedure used in the preceding example in reverse order. To begin, the indices are removed from the parentheses, and reciprocals are taken, which yields ∞ , -1 , and 1 . This means that the particular plane parallels the x axis while intersecting the y and z axes at $-b$ and c , respectively, as indicated in the accompanying sketch (a). This plane has been drawn in sketch (b). A plane is indicated by lines representing its intersections with the planes that constitute the faces of the unit cell or their extensions. For example, in this figure, line ef is the intersection between the $(0\bar{1}1)$ plane and the top face of the unit cell; also, line gh represents the intersection between



this same $(0\bar{1}1)$ plane and the plane of the bottom unit cell face extended. Similarly, lines eg and fh are the intersections between $(0\bar{1}1)$ and back and front cell faces, respectively.

ATOMIC ARRANGEMENTS

The atomic arrangement for a crystallographic plane, which is often of interest, depends on the crystal structure. The (110) atomic planes for FCC and BCC crystal structures are represented in Figures 3.9 and 3.10; reduced-sphere unit cells are also included. Note that the atomic packing is different for each case. The circles represent atoms lying in the crystallographic planes as would be obtained from a slice taken through the centers of the full-sized hard spheres.

A “family” of planes contains all those planes that are crystallographically equivalent—that is, having the same atomic packing; and a family is designated by indices that are enclosed in braces—e.g., $\{100\}$. For example, in cubic crystals the (111) , $(\bar{1}\bar{1}\bar{1})$, $(\bar{1}11)$, $(1\bar{1}\bar{1})$, $(11\bar{1})$, $(\bar{1}\bar{1}1)$, $(\bar{1}1\bar{1})$, and $(1\bar{1}1)$ planes all belong to the $\{111\}$ family. On the other hand, for tetragonal crystal structures, the $\{100\}$ family would contain only the (100) , $(\bar{1}00)$, (010) , and $(0\bar{1}0)$ since the (001) and $(00\bar{1})$ planes are not crystallographically equivalent. Also, in the cubic system only, planes having the same indices, irrespective of order and sign, are equivalent. For example, both $(1\bar{2}3)$ and $(3\bar{1}2)$ belong to the $\{123\}$ family.

HEXAGONAL CRYSTALS

For crystals having hexagonal symmetry, it is desirable that equivalent planes have the same indices; as with directions, this is accomplished by the Miller–Bravais system shown in Figure 3.6. This convention leads to the four-index $(hkil)$ scheme,

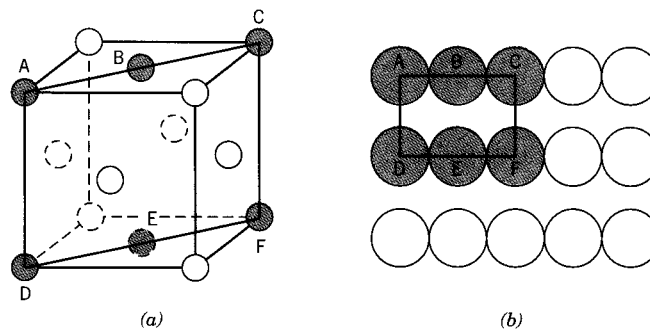
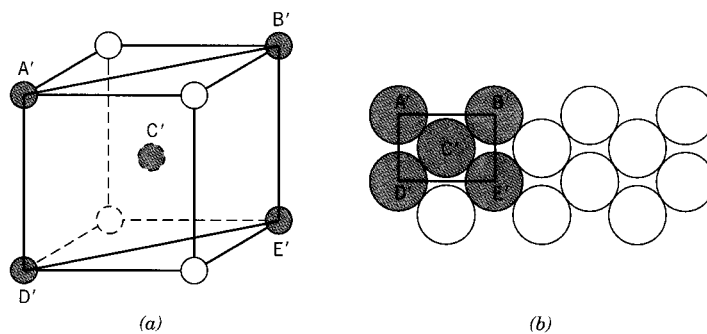


FIGURE 3.9 (a) Reduced-sphere FCC unit cell with (110) plane. (b) Atomic packing of an FCC (110) plane. Corresponding atom positions from (a) are indicated.

FIGURE 3.10 (a) Reduced-sphere BCC unit cell with (110) plane. (b) Atomic packing of a BCC (110) plane. Corresponding atom positions from (a) are indicated.



which is favored in most instances, since it more clearly identifies the orientation of a plane in a hexagonal crystal. There is some redundancy in that i is determined by the sum of h and k through

$$i = -(h + k) \quad (3.7)$$

Otherwise the three h , k , and l indices are identical for both indexing systems. Figure 3.7b presents several of the common planes that are found for crystals having hexagonal symmetry.

3.10 LINEAR AND PLANAR ATOMIC DENSITIES

The two previous sections discussed the equivalency of nonparallel crystallographic directions and planes. Directional equivalency is related to the *atomic linear density* in the sense that equivalent directions have identical linear densities. The direction vector is positioned so as to pass through atom centers, and the fraction of line length intersected by these atoms is equal to the linear density.

Correspondingly, crystallographic planes that are equivalent have the same *atomic planar density*. The plane of interest is positioned so as to pass through atom centers. And planar density is simply the fraction of total crystallographic plane area that is occupied by atoms (represented as circles). It should be noted that the concepts of linear and planar densities are one- and two-dimensional analogs of the atomic packing factor; their determinations are illustrated in the following two example problems.

EXAMPLE PROBLEM 3.8

Calculate the linear density of the $[100]$ direction for BCC.

SOLUTION

A BCC unit cell (reduced sphere) and the $[100]$ direction therein are shown in Figure 3.11a; represented in Figure 3.11b is the linear packing in this direction. As a basis for our computation let us use the line length within the unit cell, L_l , which in this case is the lattice parameter a —the distance between the centers of atoms M and N. In terms of the atomic radius R ,

$$L_l = a = \frac{4R}{\sqrt{3}} \quad (\text{see Equation 3.3})$$

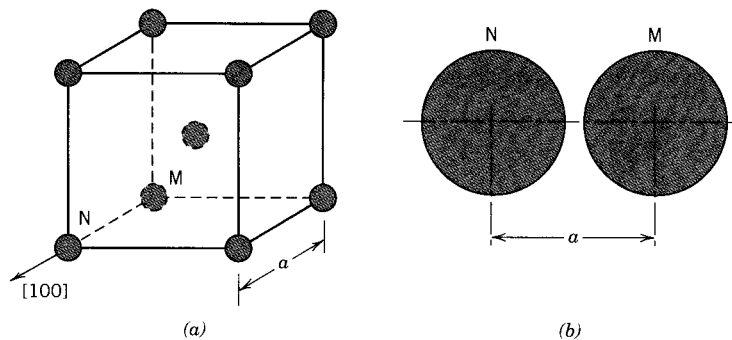


FIGURE 3.11 (a) Reduced-sphere BCC unit cell with the [100] direction indicated. (b) Atomic spacing in the [100] direction for the BCC crystal structure—between atoms M and N in (a).

Now, the total line length intersecting circles (atoms M and N), L_c , is equal to $2R$. And the linear density LD is just the following ratio:

$$LD = \frac{L_c}{L_t} = \frac{2R}{4R/\sqrt{3}} = 0.866$$

EXAMPLE PROBLEM 3.9

Calculate the planar density of the (110) plane for FCC.

SOLUTION

The atomic packing of this plane is represented in Figure 3.9b. Consider that portion of the plane that intersects a unit cell (Figure 3.9b), and then compute both this planar area and total circle area in terms of the atomic radius R . Planar density, then, is just the ratio of these two areas.

The unit cell plane area, A_p , is simply that of the rectangle circumscribed by the centers of the atoms A, C, D, and F (Figure 3.9b). The rectangle length (\overline{AC}) and width (\overline{AD}) are, respectively,

$$\begin{aligned} \overline{AC} &= 4R \\ \overline{AD} &= 2R\sqrt{2} \end{aligned} \quad \text{(see Equation 3.1)}$$

Therefore,

$$\begin{aligned} A_p &= (\overline{AC})(\overline{AD}) \\ &= (4R)(2R\sqrt{2}) = 8R^2\sqrt{2} \end{aligned}$$

Now, for the total circle area, one fourth of each of atoms A, C, D, and F and one half of atoms B and E reside within this rectangle, which gives a total of 2 equivalent circles. Thus the total circle area A_c is just

$$A_c = (2)\pi R^2$$

Finally, the planar density PD is just

$$PD = \frac{A_c}{A_p} = \frac{2\pi R^2}{8R^2\sqrt{2}} = 0.555$$