If a and c represent, respectively, the short and long unit cell dimensions of Figure 3.4*a*, the c/a ratio should be 1.633; however, for some HCP metals, this ratio deviates from the ideal value.

The coordination number and the atomic packing factor for the HCP crystal structure are the same as for FCC: 12 and 0.74, respectively. The HCP metals include cadmium, magnesium, titanium, and zinc; some of these are listed in Table 3.1.

EXAMPLE PROBLEM 3.1

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Determination of FCC Unit Cell Volume

Calculate the volume of an FCC unit cell in terms of the atomic radius R.

Solution

In the FCC unit cell illustrated, the atoms touch one another across a face-diagonal, the length of which is $4R$. Because the unit cell is a cube, its volume is a^3, where a is the cell edge length. From the right triangle on the face,

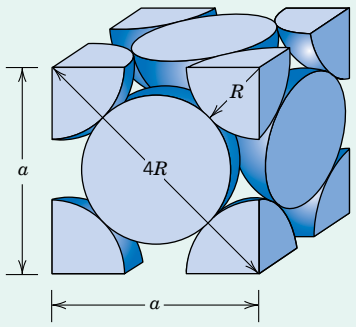
$$a^2 + a^2 = (4R)^2$$

or, solving for a,

$$a = 2R\sqrt{2} \tag{3.1}$$

The FCC unit cell volume V_C may be computed from

$$V_C = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2} \tag{3.6}$$



EXAMPLE PROBLEM 3.2

WileyPLUS
Tutorial Video

Computation of the Atomic Packing Factor for FCC

Show that the atomic packing factor for the FCC crystal structure is 0.74.

Solution

The APF is defined as the fraction of solid sphere volume in a unit cell, or

$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}} = \frac{V_S}{V_C}$$

Both the total atom and unit cell volumes may be calculated in terms of the atomic radius R. The volume for a sphere is $\frac{4}{3}\pi R^3$, and because there are four atoms per FCC unit cell, the total FCC atom (or sphere) volume is

$$V_S = (4)\tfrac{4}{3}\pi R^3 = \tfrac{16}{3}\pi R^3$$

From Example Problem 3.1, the total unit cell volume is

$$V_C = 16R^3\sqrt{2}$$

Therefore, the atomic packing factor is

$$\text{APF} = \frac{V_S}{V_C} = \frac{\left(\frac{16}{3}\right)\pi R^3}{16R^3\sqrt{2}} = 0.74$$

Concept Check 3.1

(a) What is the coordination number for the simple-cubic crystal structure?

(b) Calculate the atomic packing factor for simple cubic.

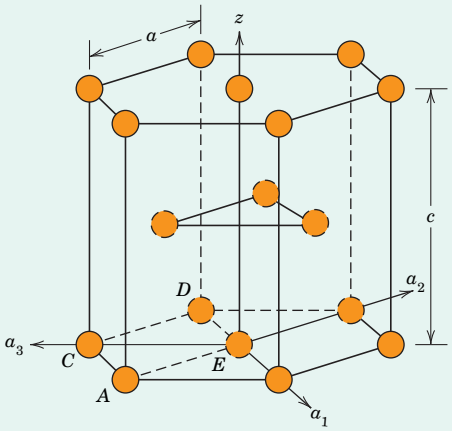
[*The answer may be found at www.wiley.com/college/callister (Student Companion Site).*]

EXAMPLE PROBLEM 3.3

Determination of HCP Unit Cell Volume

(a) Calculate the volume of an HCP unit cell in terms of its a and c lattice parameters.

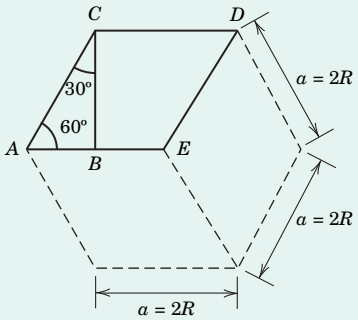
(b) Now provide an expression for this volume in terms of the atomic radius, R, and the c lattice parameter.



Solution

(a) We use the adjacent reduced-sphere HCP unit cell to solve this problem.

Now, the unit cell volume is just the product of the base area times the cell height, c. This base area is just three times the area of the parallelepiped $ACDE$ shown below. (This $ACDE$ parallelepiped is also labeled in the above unit cell.)



The area of $ACDE$ is just the length of $\overline{CD}$ times the height $\overline{BC}$. But $\overline{CD}$ is just a, and $\overline{BC}$ is equal to

$$\overline{BC} = a\cos(30°) = \frac{a\sqrt{3}}{2}$$

Thus, the base area is just

$$\text{AREA} = (3)(\overline{CD})(\overline{BC}) = (3)(a)\left(\frac{a\sqrt{3}}{2}\right) = \frac{3a^2\sqrt{3}}{2}$$

Again, the unit cell volume V_C is just the product of the AREA and c; thus,

$$\begin{aligned} V_C &= \text{AREA}(c) \\ &= \left(\frac{3a^2\sqrt{3}}{2}\right)(c) \\ &= \frac{3a^2c\sqrt{3}}{2} \end{aligned} \tag{3.7a}$$

(b) For this portion of the problem, all we need do is realize that the lattice parameter a is related to the atomic radius R as

$$a = 2R$$

Now making this substitution for a in Equation 3.7a gives

$$\begin{aligned} V_C &= \frac{3(2R)^2c\sqrt{3}}{2} \\ &= 6R^2c\sqrt{3} \end{aligned} \tag{3.7b}$$

3.5 DENSITY COMPUTATIONS

A knowledge of the crystal structure of a metallic solid permits computation of its theoretical density ρ through the relationship

Theoretical density for metals

$$\rho = \frac{nA}{V_C N_A} \tag{3.8}$$

where

n = number of atoms associated with each unit cell
A = atomic weight
V_C = volume of the unit cell
N_A = Avogadro's number (6.022×10^{23} atoms/mol)

EXAMPLE PROBLEM 3.4

Theoretical Density Computation for Copper

Copper has an atomic radius of 0.128 nm, an FCC crystal structure, and an atomic weight of 63.5 g/mol. Compute its theoretical density, and compare the answer with its measured density.

Solution

Equation 3.8 is employed in the solution of this problem. Because the crystal structure is FCC, n, the number of atoms per unit cell, is 4. Furthermore, the atomic weight A_{Cu} is given as 63.5 g/mol. The unit cell volume V_C for FCC was determined in Example Problem 3.1 as $16R^3\sqrt{2}$, where R, the atomic radius, is 0.128 nm.

Substitution for the various parameters into Equation 3.8 yields

$$\begin{aligned}\rho &= \frac{nA_{Cu}}{V_C N_A} = \frac{nA_{Cu}}{(16R^3\sqrt{2})N_A} \\ &= \frac{(4 \text{ atoms/unit cell})(63.5 \text{ g/mol})}{[16\sqrt{2}(1.28 \times 10^{-8} \text{ cm})^3/\text{unit cell}](6.022 \times 10^{23} \text{ atoms/mol})} \\ &= 8.89 \text{ g/cm}^3\end{aligned}$$

The literature value for the density of copper is 8.94 g/cm^3, which is in very close agreement with the foregoing result.

3.6 POLYMORPHISM AND ALLOTROPY

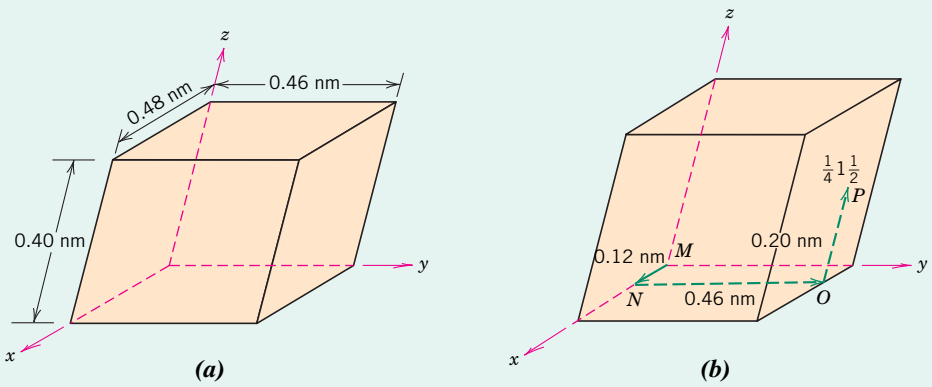
polymorphism
allotropy

Some metals, as well as nonmetals, may have more than one crystal structure, a phenomenon known as **polymorphism.** When found in elemental solids, the condition is often termed **allotropy.** The prevailing crystal structure depends on both the temperature and the external pressure. One familiar example is found in carbon: graphite is the stable polymorph at ambient conditions, whereas diamond is formed at extremely high pressures. Also, pure iron has a BCC crystal structure at room temperature, which changes to FCC iron at 912°C (1674°F). Most often a modification of the density and other physical properties accompanies a polymorphic transformation.

EXAMPLE PROBLEM 3.5

Location of Point Having Specified Coordinates

For the unit cell shown in the accompanying sketch (*a*), locate the point having coordinates $\frac{1}{4}\,1\,\frac{1}{2}$.



Solution

From sketch (*a*), edge lengths for this unit cell are as follows: $a = 0.48$ nm, $b = 0.46$ nm, and $c = 0.40$ nm. Furthermore, in light of the preceding discussion, the three point coordinate indices are $q = \frac{1}{4}$, $r = 1$, and $s = \frac{1}{2}$. We use Equations 3.9a through 3.9c to determine lattice positions for this point as follows:

$$\text{lattice position referenced to the } x \text{ axis} = qa$$
$$= \left(\tfrac{1}{4}\right)a = \tfrac{1}{4}(0.48\text{ nm}) = 0.12\text{ nm}$$

$$\text{lattice position referenced to the } y \text{ axis} = rb$$
$$= (1)b = (1)(0.46\text{ nm}) = 0.46\text{ nm}$$

$$\text{lattice position referenced to the } z \text{ axis} = sc$$
$$= \left(\tfrac{1}{2}\right)c = \left(\tfrac{1}{2}\right)(0.40\text{ nm}) = 0.20\text{ nm}$$

To locate the point having these coordinates within the unit cell, first use the x lattice position and move from the origin (point M) 0.12 nm units along the x axis (to point N), as shown in (*b*). Similarly, using the y lattice position, proceed 0.46 nm parallel to the y axis, from point N to point O. Finally, move from this position 0.20 nm units parallel to the z axis to point P (per the z lattice position), as noted again in (*b*). Thus, point P corresponds to the $\frac{1}{4}\,1\,\frac{1}{2}$ point coordinates.

EXAMPLE PROBLEM 3.6

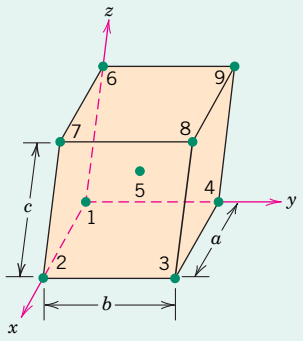
Specification of Point Coordinate Indices

Specify coordinate indices for all numbered points of the unit cell in the illustration on the next page.

Solution

For this unit cell, coordinate points are located at all eight corners with a single point at the center position.

Point 1 is located at the origin of the coordinate system, and, therefore, its lattice position indices referenced to the x, y, and z axes are $0a$, $0b$, and $0c$, respectively. And from Equations 3.9a through 3.9c,



$$\text{lattice position referenced to the } x \text{ axis} = 0a = qa$$
$$\text{lattice position referenced to the } y \text{ axis} = 0b = rb$$
$$\text{lattice position referenced to the } z \text{ axis} = 0c = sc$$

Solving the above three expressions for values of the q, r, and s indices leads to

$$q = \frac{0a}{a} = 0$$
$$r = \frac{0b}{b} = 0$$
$$s = \frac{0c}{c} = 0$$

Therefore this is the 0 0 0 point

Because point number 2, lies one unit cell edge length along the x axis, its lattice position indices referenced to the x, y, and z axes are a, $0b$, and $0c$, and

$$\text{lattice position index referenced to the } x \text{ axis} = a = qa$$
$$\text{lattice position index referenced to the } y \text{ axis} = 0b = rb$$
$$\text{lattice position index referenced to the } z \text{ axis} = 0c = sc$$

Thus we determine values for the q, r, and s indices as follows:

$$q = 1 \qquad r = 0 \qquad s = 0$$

Hence, point 2 is 1 0 0.

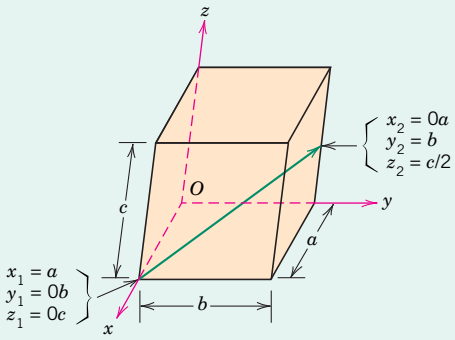
This same procedure is carried out for the remaining seven points in the unit cell. Point indices for all nine points are listed in the following table.

Point Number	q	r	s
1	0	0	0
2	1	0	0
3	1	1	0
4	0	1	0
5	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
6	0	0	1
7	1	0	1
8	1	1	1
9	0	1	1

EXAMPLE PROBLEM 3.7

Determination of Directional Indices

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



Solution

It is first necessary to take note of the vector tail and head coordinates. From the illustration, tail coordinates are as follows:

$$x_1 = a \qquad y_1 = 0b \qquad z_1 = 0c$$

For the head coordinates,

$$x_2 = 0a \qquad y_2 = b \qquad z_2 = c/2$$

Now taking point coordinate differences,

$$x_2 - x_1 = 0a - a = -a$$
$$y_2 - y_1 = b - 0b = b$$
$$z_2 - z_1 = c/2 - 0c = c/2$$

It is now possible to use Equations 3.10a through 3.10c to compute values of u, v, and w. However, because the $z_2 - z_1$ difference is a fraction (i.e., $c/2$), we anticipate that in order to have integer values for the three indices, it is necessary to assign n a value of 2. Thus,

$$u = n\left(\frac{x_2 - x_1}{a}\right) = 2\left(\frac{-a}{a}\right) = -2$$
$$v = n\left(\frac{y_2 - y_1}{b}\right) = 2\left(\frac{b}{b}\right) = 2$$
$$w = n\left(\frac{z_2 - z_1}{c}\right) = 2\left(\frac{c/2}{c}\right) = 1$$

And, finally enclosure of the -2, 2, and 1 indices in brackets leads to $[\bar{2}21]$ as the direction designation.[4]

This procedure is summarized as follows:

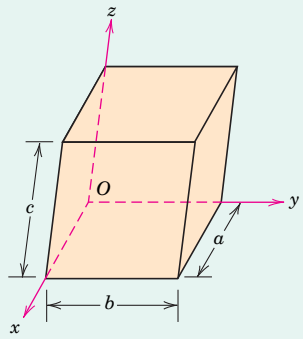
	x	*y*	*z*
Head coordinates (x_2, y_2, z_2,)	$0a$	b	$c/2$
Tail coordinates (x_1, y_1, z_1,)	a	$0b$	$0c$
Coordinate differences	$-a$	b	$c/2$
Calculated values of u, v, and w	$u = -2$	$v = 2$	$w = 1$
Enclosure		$[\bar{2}21]$	

[4]If these u, v, and w values are not integers, it is necessary to choose another value for n.

EXAMPLE PROBLEM 3.8

Construction of a Specified Crystallographic Direction

Within the following unit cell draw a $[1\bar{1}0]$ direction with its tail located at the origin of the coordinate system, point O.



Solution

This problem is solved by reversing the procedure of the preceding example. For this $[1\bar{1}0]$ direction,

$$u = 1$$
$$v = -1$$
$$w = 0$$

Because the tail of the direction vector is positioned at the origin, its coordinates are as follows:

$$x_1 = 0a$$
$$y_1 = 0b$$
$$z_1 = 0c$$

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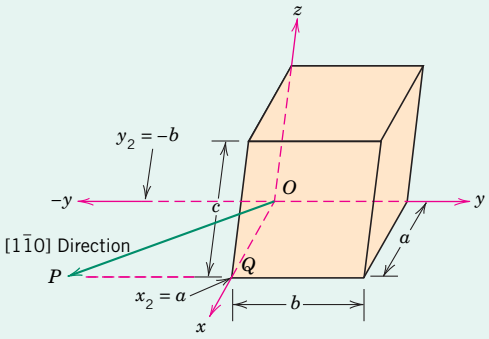
We now want to solve for the coordinates of the vector head—that is, x_2, y_2, and z_2. This is possible using rearranged forms of Equations 3.10a through 3.10c and incorporating the above values for the three direction indices (u, v, and w) and vector tail coordinates. Taking the value of n to be 1 because the three direction indices are all integers leads to

$$x_2 = ua + x_1 = (1)(a) + 0a = a$$
$$y_2 = vb + y_1 = (-1)(b) + 0b = -b$$
$$z_2 = wc + z_1 = (0)(c) + 0c = 0c$$

The construction process for this direction vector is shown in the following figure.



Because the tail of the vector is positioned at the origin, we start at the point labeled O and then move in a stepwise manner to locate the vector head. Because the x head coordinate (x_2) is a, we proceed from point O, a units along the x axis to point Q. From point Q, we move b units parallel to the $-y$ axis to point P, because the y head coordinate (y_2) is $-b$. There is no z component to the vector inasmuch as the z head coordinate (z_2) is $0c$. Finally, the vector corresponding to this $[1\bar{1}0]$ direction is constructed by drawing a line from point O to point P, as noted in the illustration.

For some crystal structures, several nonparallel directions with different indices are *crystallographically equivalent*, meaning 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 is enclosed in angle

EXAMPLE PROBLEM 3.9

Conversion and Construction of Directional Indices for a Hexagonal Unit Cell

(a) Convert the [111] direction into the four-index system for hexagonal crystals.
(b) Draw this direction within a ruled-net coordinate system (per Figure 3.10).
(c) Now draw the [111] direction within a hexagonal unit cell that utilizes a three-axis (a_1, a_2, z) coordinate scheme.

Solution

(a) This conversion is carried out using Equations 3.11a–3.11d, in which

$$U = 1 \qquad V = 1 \qquad W = 1$$

Thus,

$$u = \frac{1}{3}(2U - V) = \frac{1}{3}[(2)(1) - 1] = \frac{1}{3}$$

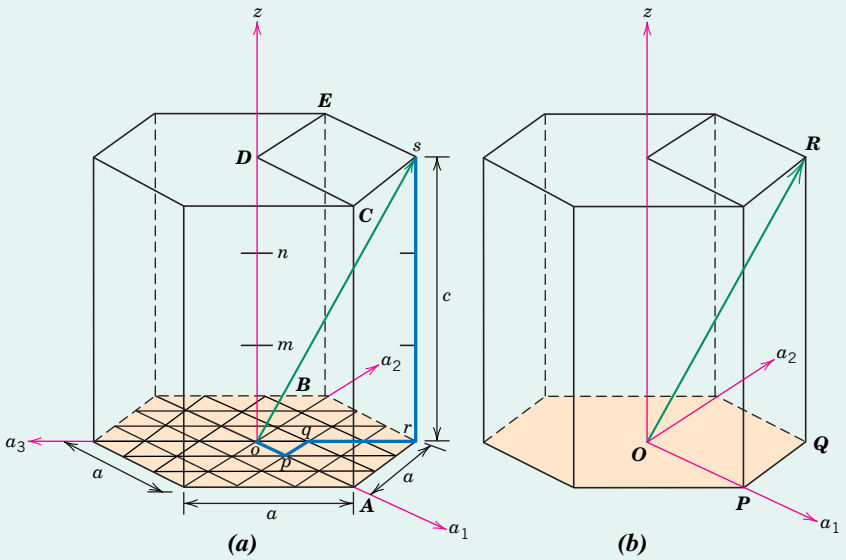
$$v = \frac{1}{3}(2V - U) = \frac{1}{3}[(2)(1) - 1] = \frac{1}{3}$$

$$t = -(u + v) = -\left(\frac{1}{3} + \frac{1}{3}\right) = -\frac{2}{3}$$

$$w = W = 1$$

Multiplication of the preceding indices by 3 reduces them to the lowest set, which yields values for u, v, t, and w of 1, 1, −2, and 3, respectively. Hence, the [111] direction becomes $[11\bar{2}3]$.

(b) The following sketch (a) shows a hexagonal unit cell in which the ruled-net coordinate system has been drawn.



Also, one of the three parallelepipeds that makes up the hexagonal cell is delineated—its corners are labeled with letters *o*-*A*-*r*-*B*-*C*-*D*-*E*-*s*, with the origin of the a_1-a_2-a_3-z axis coordinate system located at the corner labeled *o*. It is within this unit cell that we draw the $[11\bar{2}3]$ direction. For the sake of convenience, let us position the vector tail at the origin of the coordinate system, which means that $a_1'' = a_2'' = a_3'' = 0a$ and $z'' = 0c$. Coordinates for

the vector head (a_1', a_2', a_3', and z') may be determined using rearranged forms of Equations 3.12a–3.12d, taking the value of n to be unity. Thus,

$$a_1' = \frac{ua}{3n} + a_1'' = \frac{(1)(a)}{(3)(1)} + 0a = \frac{a}{3}$$

$$a_2' = \frac{va}{3n} + a_2'' = \frac{(1)(a)}{(3)(1)} + 0a = \frac{a}{3}$$

$$a_3' = \frac{ta}{3n} + a_3'' = \frac{(-2)(a)}{(3)(1)} + 0a = \frac{-2a}{3}$$

$$z' = \frac{wc}{3n} + z'' = \frac{(3)(c)}{(3)(1)} + 0c = c$$

In constructing this direction vector, we begin at the origin (point o), and first proceed $\frac{a}{3}$ units along the a_1 axis to point p; next, from this point parallel to the a_2 axis $\frac{a}{3}$ units to point q; then parallel to the a_3 axis $-\frac{2a}{3}$ units to point r; and finally we continue parallel to the z axis c units to point s. Thus, the $[11\bar{2}3]$ direction is represented by the vector that is directed from point o to point s, as noted in the sketch.

(c) Of course, it is possible to draw the equivalent [111] direction using a three-coordinate-axis (a_1-a_2-z) technique, as shown in (b). In this case, we modify Equations 3.10a–3.10c to read as follows:

$$U = n\left(\frac{a_1' - a_1''}{a}\right) \tag{3.13a}$$

$$V = n\left(\frac{a_2' - a_2''}{a}\right) \tag{3.13b}$$

$$W = n\left(\frac{z' - z''}{c}\right) \tag{3.13c}$$

where again, single and double primes for a_1, a_2, and z denote head and tail coordinates, respectively. When we locate tail coordinates at the origin (i.e., take $a_1'' = a_2'' = 0a$ and $z'' = 0c$) and make the vector head (i.e., single-primed) coordinates of the above equations dependent parameters (while assuming $n = 1$), the following result:

$$a_1' = \frac{Ua}{n} + a_1'' = \frac{(1)(a)}{(1)} + 0a = a$$

$$a_2' = \frac{Va}{n} + a_2'' = \frac{(1)(a)}{(1)} + 0a = a$$

$$z' = \frac{Wc}{n} + z'' = \frac{(1)(c)}{(1)} + 0c = c$$

To locate the vector head, we begin at the origin (point O), then proceed a units along the a_1 axis (to point P), next parallel to the a_2 axis a units (to point Q), and finally parallel to the z axis c units (to point R). Hence, the [111] direction is represented by the vector that passes from O to R, as shown.

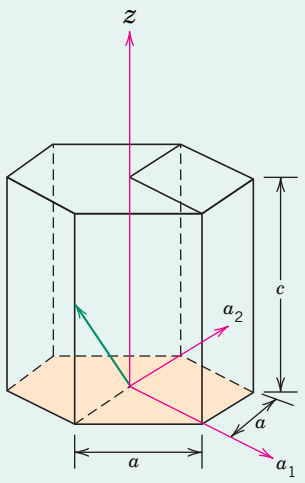
It may be noted that this [111] direction is identical to $[11\bar{2}3]$ from part (b).

The alternative situation is to determine the indices for a direction that has been drawn within a hexagonal unit cell. For this case, it is convenient to use the a_1-a_2-z three-coordinate-axis system and then convert these indices into the equivalent set for the four-axis scheme. The following example problem demonstrates this procedure.

EXAMPLE PROBLEM 3.10

Determination of Directional Indices for a Hexagonal Unit Cell

Determine the indices (four-index system) for the direction shown in the accompanying figure.



Solution

The first thing we need to do is determine U, V, and W indices for the vector referenced to the three-axis scheme represented in the sketch; this is possible using Equations 3.13a through 3.13c. Because the vector passes through the origin, $a_1'' = a_2'' = 0a$ and $z'' = 0c$. Furthermore, from the sketch, coordinates for the vector head are as follows:

$$a_1' = 0a$$
$$a_2' = -a$$
$$z' = \frac{c}{2}$$

Because the denominator in z' is 2, we assume that $n = 2$. Therefore,

$$U = n\left(\frac{a_1' - a_1''}{a}\right) = 2\left(\frac{0a - 0a}{a}\right) = 0$$
$$V = n\left(\frac{a_2' - a_2''}{a}\right) = 2\left(\frac{-a - 0a}{a}\right) = -2$$
$$W = n\left(\frac{z' - z''}{c}\right) = 2\left(\frac{c/2 - 0c}{c}\right) = 1$$

This direction is represented by enclosing the above indices in brackets—namely, $[0\bar{2}1]$.

Now it becomes necessary to convert these indices into an index set referenced to the four-axis scheme. This requires the use of Equations 3.11a–3.11d. For this $[0\bar{2}1]$ direction,

$$U = 0 \qquad V = -2 \qquad W = 1$$

and

$$u = \frac{1}{3}(2U - V) = \frac{1}{3}[(2)(0) - (-2)] = \frac{2}{3}$$
$$v = \frac{1}{3}(2V - U) = \frac{1}{3}[(2)(-2) - 0] = -\frac{4}{3}$$
$$t = -(u + v) = -\left(\frac{2}{3} - \frac{4}{3}\right) = \frac{2}{3}$$
$$w = W = 1$$

Multiplication of the preceding indices by 3 reduces them to the lowest set, which yields values for u, v, t, and w of 2, −4, 2, and 3, respectively. Hence, the direction vector shown in the figure is $[2\bar{4}23]$.

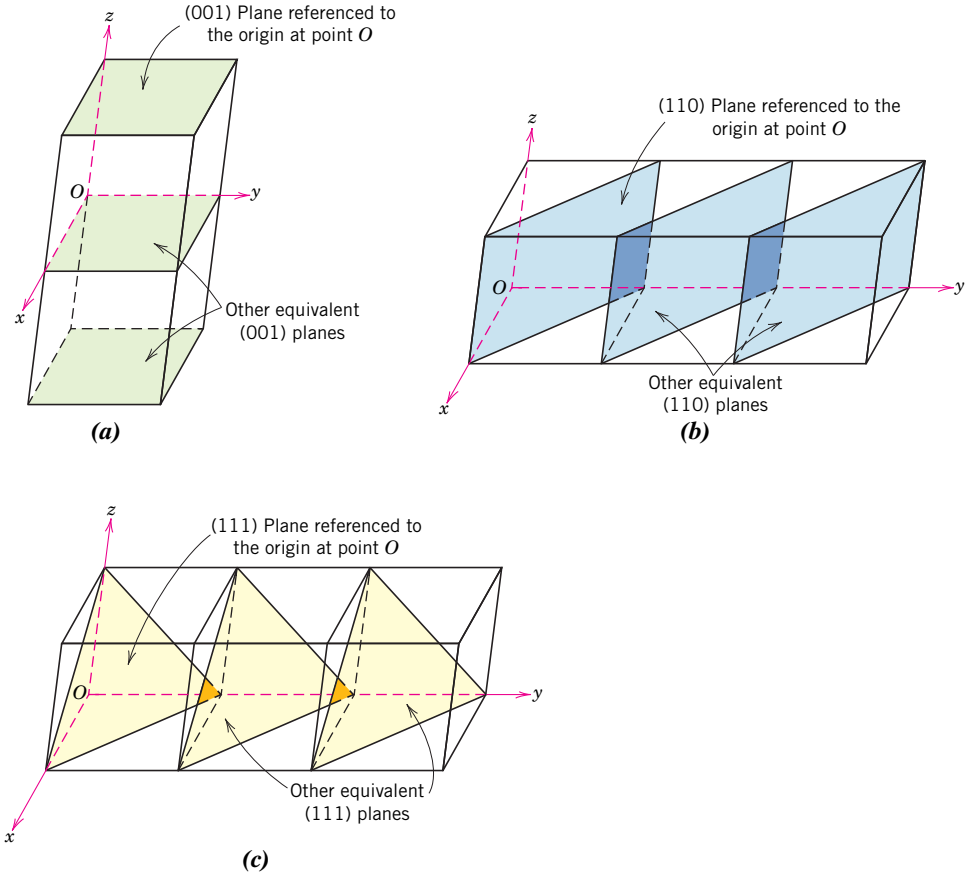


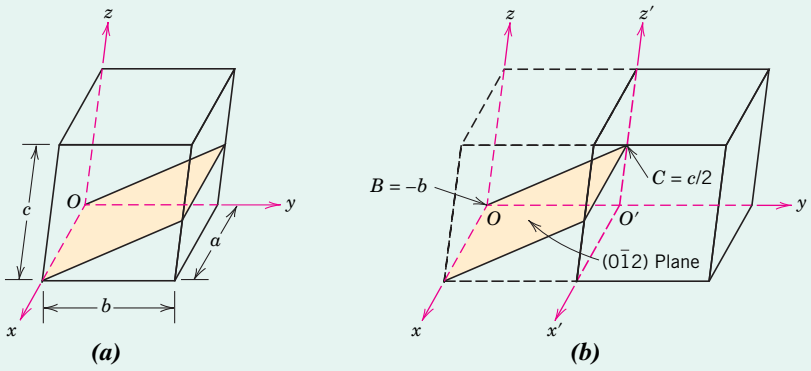
Figure 3.11 Representations of a series each of the (*a*) (001), (*b*) (110), and (*c*) (111) crystallographic planes.

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.

EXAMPLE PROBLEM 3.11

Determination of Planar (Miller) Indices

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



Solution

Because the plane passes through the selected origin O, a new origin must be chosen at the corner of an adjacent unit cell. In choosing this new unit cell, we move one unit-cell distance parallel to the y-axis, as shown in sketch (b). Thus x'-y-z' is the new coordinate axis system having its origin located at O'. Because this plane is parallel to the x' axis its intercept is ∞a—that is, $A = \infty a$. Furthermore, from illustration (b), intersections with the y and z' axes are as follows:

$$B = -b \qquad C = c/2$$

It is now possible to use Equations 3.14a–3.14c to determine values of h, k, and l. At this point, let us choose a value of 1 for n. Thus,

$$h = \frac{na}{A} = \frac{1a}{\infty a} = 0$$

$$k = \frac{nb}{B} = \frac{1b}{-b} = -1$$

$$l = \frac{nc}{C} = \frac{1c}{c/2} = 2$$

And finally, enclosure of the 0, −1, and 2 indices in parentheses leads to $(0\bar{1}2)$ as the designation for this direction.[8]

This procedure is summarized as follows:

	x	*y*	*z*
Intercepts (A, B, C)	∞a	$-b$	$c/2$
Calculated values of h, k, and l (Equations 3.14a–3.14c)	$h = 0$	$k = -1$	$l = 2$
Enclosure		$(0\bar{1}2)$	

EXAMPLE PROBLEM 3.12

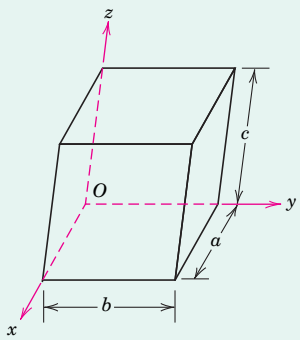
Construction of a Specified Crystallographic Plane

Construct a (101) plane within the following unit cell.

Solution

To solve this problem, carry out the procedure used in the preceding example in reverse order. For this (101) direction,

$$h = 1$$
$$k = 0$$
$$l = 1$$



(a)

[8]If h, k, and l are not integers, it is necessary to choose another value for n.