ch03 Solution Manual Material Science and Engineering 8th Edition

Materials science

Hitec University (HU)

97 pag.

THE STRUCTURE OF CRYSTALLINE SOLIDS

PROBLEM SOLUTIONS

Fundamental Concepts

3.1 What is the difference between atomic structure and crystal structure?

<u>Solution</u>

Atomic structure relates to the number of protons and neutrons in the nucleus of an atom, as well as the number and probability distributions of the constituent electrons. On the other hand, crystal structure pertains to the arrangement of atoms in the crystalline solid material.

<center>**Unit Cells**</center>
<center>**Metallic Crystal Structures**</center>

3.2 If the atomic radius of aluminum is 0.143 nm, calculate the volume of its unit cell in cubic meters.
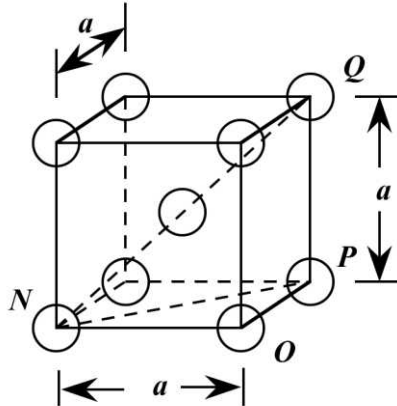
<u>Solution</u>

For this problem, we are asked to calculate the volume of a unit cell of aluminum. Aluminum has an FCC crystal structure (Table 3.1). The FCC unit cell volume may be computed from Equation 3.4 as

$$V_C = 16R^3\sqrt{2} = (16)(0.143 \times 10^{-9} \text{ m})^3(\sqrt{2}) = 6.62 \times 10^{-29} \text{ m}^3$$

3.3 Show for the body-centered cubic crystal structure that the unit cell edge length a and the atomic radius R are related through a $= 4R/\sqrt{3}$.

Consider the BCC unit cell shown below

Using the triangle NOP

$$(\overline{NP})^2 = a^2 + a^2 = 2a^2$$

And then for triangle NPQ,

$$(\overline{NQ})^2 = (\overline{QP})^2 + (\overline{NP})^2$$

But $\overline{NQ} = 4R$, R being the atomic radius. Also, $\overline{QP} = a$. Therefore,
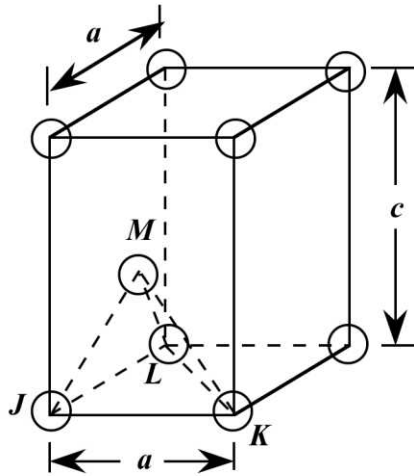
$$(4R)^2 = a^2 + 2a^2$$
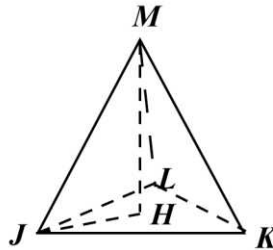
or

$$a = \frac{4R}{\sqrt{3}}$$

3.4 For the HCP crystal structure, show that the ideal c/a ratio is 1.633.

A sketch of one-third of an HCP unit cell is shown below.

Consider the tetrahedron labeled as JKLM, which is reconstructed as

The atom at point M is midway between the top and bottom faces of the unit cell--that is $\overline{MH}$ = c/2. And, since atoms at points J, K, and M, all touch one another,

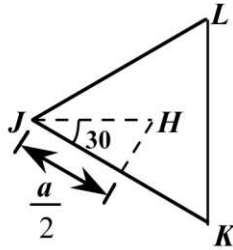$$\overline{JM} = \overline{JK} = 2R = a$$

where R is the atomic radius. Furthermore, from triangle JHM,

$$(\overline{JM})^2 = (\overline{JH})^2 + (\overline{MH})^2$$

or

$$a^2 = (\overline{JH})^2 + \left(\frac{c}{2}\right)^2$$

Now, we can determine the $\overline{JH}$ length by consideration of triangle JKL, which is an equilateral triangle,

$$\cos 30° = \frac{a/2}{JH} = \frac{\sqrt{3}}{2}$$

and

$$\overline{JH} = \frac{a}{\sqrt{3}}$$

Substituting this value for $\overline{JH}$ in the above expression yields

$$a^2 = \left(\frac{a}{\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)^2 = \frac{a^2}{3} + \frac{c^2}{4}$$

and, solving for c/a

$$\frac{c}{a} = \sqrt{\frac{8}{3}} = 1.633$$

3.5 Show that the atomic packing factor for BCC is 0.68.

<u>Solution</u>

The atomic packing factor is defined as the ratio of sphere volume to the total unit cell volume, or

$$APF = \frac{V_S}{V_C}$$

Since there are two spheres associated with each unit cell for BCC

$$V_S = 2(\text{sphere volume}) = 2\left(\frac{4\pi R^3}{3}\right) = \frac{8\pi R^3}{3}$$

Also, the unit cell has cubic symmetry, that is $V_C = a^3$. But a depends on R according to Equation 3.3, and

$$V_C = \left(\frac{4R}{\sqrt{3}}\right)^3 = \frac{64\,R^3}{3\sqrt{3}}$$

Thus,

$$APF = \frac{V_S}{V_C} = \frac{8\pi\,R^3/3}{64\,R^3/3\sqrt{3}} = 0.68$$

3.6 Show that the atomic packsing factor for HCP is 0.74.

The APF is just the total sphere volume-unit cell volume ratio. For HCP, there are the equivalent of six spheres per unit cell, and thus

$$V_S = 6\left(\frac{4\pi R^3}{3}\right) = 8\pi R^3$$

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.
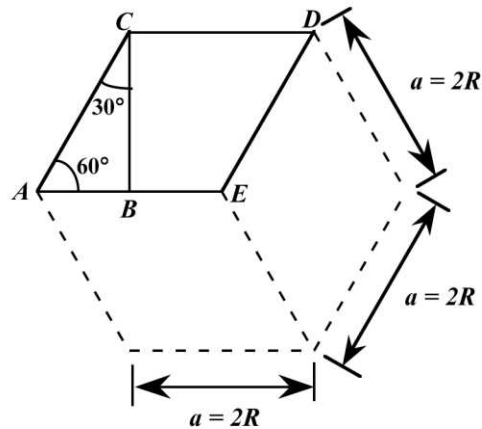
The area of ACDE is just the length of $\overline{CD}$ times the height $\overline{BC}$. But $\overline{CD}$ is just a or 2R, and

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

Thus, the base area is just

$$AREA = (3)(\overline{CD})(\overline{BC}) = (3)(2R)\left(\frac{2R\sqrt{3}}{2}\right) = 6R^2\sqrt{3}$$

and since c = 1.633a = 2R(1.633)

$$V_C = (AREA)(c) = 6R^2c\sqrt{3} \tag{3.S1}$$

$$= \left(6 R^2 \sqrt{3} \right) (2)(1.633)R = 12\sqrt{3}(1.633)R^3$$

Thus,

$$APF = \frac{V_S}{V_C} = \frac{8\pi R^3}{12\sqrt{3}(1.633)R^3} = 0.74$$

Density Computations

3.7 Iron has a BCC crystal structure, an atomic radius of 0.124 nm, and an atomic weight of 55.85 g/mol. Compute and compare its theoretical density with the experimental value found inside the front cover.

Solution

This problem calls for a computation of the density of iron. According to Equation 3.5

$$\rho = \frac{nA_{Fe}}{V_C N_A}$$

For BCC, n = 2 atoms/unit cell, and

$$V_C = \left(\frac{4R}{\sqrt{3}}\right)^3$$

Thus,

$$\rho = \frac{nA_{Fe}}{\left(\dfrac{4R}{\sqrt{3}}\right)^3 N_A}$$

$$= \frac{(2 \text{ atoms/unit cell})(55.85 \text{ g/mol})}{\left[(4)\left(0.124 \times 10^{-7} \text{ cm}\right)/\sqrt{3}\right]^3/(\text{unit cell})\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}$$

$$= 7.90 \text{ g/cm}^3$$

The value given inside the front cover is 7.87 g/cm^3.

3.8 Calculate the radius of an iridium atom, given that Ir has an FCC crystal structure, a density of 22.4 g/cm^3, and an atomic weight of 192.2 g/mol.

<u>Solution</u>

We are asked to determine the radius of an iridium atom, given that Ir has an FCC crystal structure. For FCC, n = 4 atoms/unit cell, and $V_C = 16R^3\sqrt{2}$ (Equation 3.4). Now,

$$\rho = \frac{nA_{Ir}}{V_C N_A}$$

$$= \frac{nA_{Ir}}{(16R^3\sqrt{2})N_A}$$

And solving for R from the above expression yields

$$R = \left(\frac{nA_{Ir}}{16\rho N_A \sqrt{2}}\right)^{1/3}$$

$$= \left[\frac{(4\text{ atoms/unit cell})(192.2\text{ g/mol})}{(16)(22.4\text{ g/cm}^3)(6.022 \times 10^{23}\text{ atoms/mol})(\sqrt{2})}\right]^{1/3}$$

$$= 1.36 \times 10^{-8}\text{ cm} = 0.136\text{ nm}$$

3.9 Calculate the radius of a vanadium atom, given that V has a BCC crystal structure, a density of 5.96 g/cm^3, and an atomic weight of 50.9 g/mol.

This problem asks for us to calculate the radius of a vanadium atom. For BCC, n = 2 atoms/unit cell, and

$$V_C = \left(\frac{4R}{\sqrt{3}}\right)^3 = \frac{64\,R^3}{3\sqrt{3}}$$

Since, from Equation 3.5

$$\rho = \frac{nA_V}{V_C\,N_A}$$

$$= \frac{nA_V}{\left(\dfrac{64\,R^3}{3\sqrt{3}}\right)N_A}$$

and solving for R the previous equation

$$R = \left(\frac{3\sqrt{3}nA_V}{64\,\rho\,N_A}\right)^{1/3}$$

and incorporating values of parameters given in the problem statement

$$R = \left[\frac{\left(3\sqrt{3}\right)(2 \text{ atoms/unit cell})\,(50.9 \text{ g/mol})}{(64)\left(5.96 \text{ g/cm}^3\right)\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}\right]^{1/3}$$

$$= 1.32 \times 10^{-8} \text{ cm} = 0.132 \text{ nm}$$

3.10   Some hypothetical metal has the simple cubic crystal structure shown in Figure 3.24. If its atomic weight is 70.4 g/mol and the atomic radius is 0.126 nm, compute its density.

For the simple cubic crystal structure, the value of n in Equation 3.5 is unity since there is only a single atom associated with each unit cell. Furthermore, for the unit cell edge length, a = 2R (Figure 3.24). Therefore, employment of Equation 3.5 yields

$$\rho \;=\; \frac{nA}{V_C N_A} \;=\; \frac{nA}{(2\,R)^3 N_A}$$

and incorporating values of the other parameters provided in the problem statement leads to

$$\rho = \frac{(1 \text{ atom/unit cell})(70.4 \text{ g/mol})}{\left\{\left[(2)\left(1.26 \times 10^{-8} \text{ cm}\right)\right]^3 / (\text{unit cell})\right\}\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}$$

$$7.31 \text{ g/cm}^3$$

3.11 Zirconium has an HCP crystal structure and a density of 6.51 g/cm^3.

(a) What is the volume of its unit cell in cubic meters?

(b) If the c/a ratio is 1.593, compute the values of c and a.

<u>Solution</u>

(a) The volume of the Zr unit cell may be computed using Equation 3.5 as

$$V_C = \frac{nA_{Zr}}{\rho N_A}$$

Now, for HCP, n = 6 atoms/unit cell, and for Zr, A_{Zr} = 91.22 g/mol. Thus,

$$V_C = \frac{(6 \text{ atoms/unit cell})(91.22 \text{ g/mol})}{\left(6.51 \text{ g/cm}^3\right)\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}$$

$$= 1.396 \times 10^{-22} \text{ cm}^3/\text{unit cell} = 1.396 \times 10^{-28} \text{ m}^3/\text{unit cell}$$

(b) From Equation 3.S1 of the solution to Problem 3.6, for HCP

$$V_C = 6R^2 c\sqrt{3}$$

But, since a = 2R, (i.e., R = a/2) then

$$V_C = 6\left(\frac{a}{2}\right)^2 c\sqrt{3} = \frac{3\sqrt{3}\,a^2 c}{2}$$

but, since c = 1.593a

$$V_C = \frac{3\sqrt{3}\,(1.593)\,a^3}{2} = 1.396 \times 10^{-22} \text{ cm}^3/\text{unit cell}$$

Now, solving for a

$$a = \left[\frac{(2)\left(1.396 \times 10^{-22} \text{ cm}^3\right)}{(3)\left(\sqrt{3}\right)(1.593)}\right]^{1/3}$$

$$= 3.23 \times 10^{-8} \text{ cm} = 0.323 \text{ nm}$$

And finally

$$c = 1.593a = (1.593)(0.323 \text{ nm}) = 0.515 \text{ nm}$$

3.12 Using atomic weight, crystal structure, and atomic radius data tabulated inside the front cover, compute the theoretical densities of lead, chromium, copper, and cobalt, and then compare these values with the measured densities listed in this same table. The c/a ratio for cobalt is 1.623.

Solution

Since Pb has an FCC crystal structure, n = 4, and $V_C = 16R^3\sqrt{2}$ (Equation 3.4). Also, R = 0.175 nm (1.75 × 10^{-8} cm) and A_{Pb} = 207.2 g/mol. Employment of Equation 3.5 yields

$$\rho = \frac{nA_{Pb}}{V_C N_A}$$

$$= \frac{(4 \text{ atoms/unit cell})(207.2 \text{ g/mol})}{\left\{\left[(16)\left(1.75 \times 10^{-8} \text{ cm}\right)^3\left(\sqrt{2}\right)\right]/(\text{unit cell})\right\}\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}$$

$$= 11.35 \text{ g/cm}^3$$

The value given in the table inside the front cover is 11.35 g/cm^3.

Chromium has a BCC crystal structure for which n = 2 and $V_C = a^3 = \left(\frac{4R}{\sqrt{3}}\right)^3$ (Equation 3.3). Also A_{Cr} = 52.00 g/mol and R = 0.125 nm. Therefore, employment of Equation 3.5 leads to

$$\rho = \frac{(2 \text{ atoms/unit cell})(52.00 \text{ g/mol})}{\left\{\left[\frac{(4)\left(1.25 \times 10^{-8} \text{ cm}\right)}{\sqrt{3}}\right]^3/(\text{unit cell})\right\}\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}$$

$$= 7.18 \text{ g/cm}^3$$

The value given in the table is 7.19 g/cm^3.

Copper also has an FCC crystal structure and therefore

$$\rho = \frac{(4 \text{ atoms/unit cell})(63.55 \text{ g/mol})}{\left\{\left[(2)\left(1.28 \times 10^{-8} \text{ cm}\right)(\sqrt{2})\right]^3/(\text{unit cell})\right\}\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}$$

$$= 8.90 \text{ g/cm}^3$$

The value given in the table is 8.90 g/cm^3.

Cobalt has an HCP crystal structure, and from the solution to Problem 3.6 (Equation 3.S1),

$$V_C = 6R^2 c\sqrt{3}$$

and, since c = 1.623a and a = 2R, c = (1.623)(2R); hence

$$V_C = 6R^2(1.623)(2R)\sqrt{3} = (19.48)(\sqrt{3})R^3$$

$$= (19.48)(\sqrt{3})(1.25 \times 10^{-8} \text{ cm})^3$$

$$= 6.59 \times 10^{-23} \text{ cm}^3/\text{unit cell}$$

Also, there are 6 atoms/unit cell for HCP. Therefore the theoretical density is

$$\rho = \frac{nA_{Co}}{V_C N_A}$$

$$= \frac{(6 \text{ atoms/unit cell})(58.93 \text{ g/mol})}{\left(6.59 \times 10^{-23} \text{ cm}^3/\text{unit cell}\right)\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}$$

$$= 8.91 \text{ g/cm}^3$$

The value given in the table is 8.9 g/cm^3.

3.13 Rhodium has an atomic radius of 0.1345 nm and a density of 12.41 g/cm^3. Determine whether it has an FCC or BCC crystal structure.

In order to determine whether Rh has an FCC or a BCC crystal structure, we need to compute its density for each of the crystal structures. For FCC, n = 4, and a = $2R\sqrt{2}$ (Equation 3.1). Also, from Figure 2.6, its atomic weight is 102.91 g/mol. Thus, for FCC (employing Equation 3.5)

$$\rho \ = \ \frac{nA_{Rh}}{a^3 N_A} \ = \ \frac{nA_{Rh}}{(2R\sqrt{2})^3 N_A}$$

$$= \frac{(4 \text{ atoms/unit cell})(102.91 \text{ g/mol})}{\left\{\left[(2)(1.345 \ \times \ 10^{-8} \text{ cm})(\sqrt{2})\right]^3 /(\text{unit cell})\right\}(6.022 \ \times \ 10^{23} \text{ atoms}/\text{mol})}$$

$$= 12.41 \text{ g/cm}^3$$

which is the value provided in the problem statement. Therefore, Rh has the FCC crystal structure.

3.14   Below are listed the atomic weight, density, and atomic radius for three hypothetical alloys. For each determine whether its crystal structure is FCC, BCC, or simple cubic and then justify your determination. A simple cubic unit cell is shown in Figure 3.24.

Alloy	Atomic Weight (g/mol)	Density (g/cm^3)	Atomic Radius (nm)
A	77.4	8.22	0.125
B	107.6	13.42	0.133
C	127.3	9.23	0.142

Solution

For each of these three alloys we need, by trial and error, to calculate the density using Equation 3.5, and compare it to the value cited in the problem. For SC, BCC, and FCC crystal structures, the respective values of n are 1, 2, and 4, whereas the expressions for a (since $V_C = a^3$) are 2R, $2R\sqrt{2}$, and $\dfrac{4R}{\sqrt{3}}$.

For alloy A, let us calculate ρ assuming a simple cubic crystal structure.

$$\rho = \frac{nA_A}{V_C N_A}$$

$$= \frac{nA_A}{(2R)^3 N_A}$$

$$= \frac{(1\text{ atom/unit cell})(77.4\text{ g/mol})}{\left\{\left[(2)(1.25 \times 10^{-8})\right]^3/(\text{unit cell})\right\}\left(6.022 \times 10^{23}\text{ atoms/mol}\right)}$$

$$= 8.22\text{ g/cm}^3$$

Therefore, its crystal structure is simple cubic.

For alloy B, let us calculate ρ assuming an FCC crystal structure.

$$\rho = \frac{nA_B}{(2R\sqrt{2})^3 N_A}$$

$$= \frac{(4 \text{ atoms/unit cell})(107.6 \text{ g/mol})}{\left\{\left[\left(2\sqrt{2}\right)\left(1.33 \times 10^{-8} \text{ cm}\right)\right]^3 /(\text{unit cell})\right\}\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}$$

$$= 13.42 \text{ g/cm}^3$$

Therefore, its crystal structure is FCC.

For alloy C, let us calculate ρ assuming a simple cubic crystal structure.

$$= \frac{nA_C}{(2R)^3 N_A}$$

$$= \frac{(1 \text{ atom/unit cell})(127.3 \text{ g/mol})}{\left\{\left[(2)\left(1.42 \times 10^{-8} \text{ cm}\right)\right]^3 /(\text{unit cell})\right\}\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}$$

$$= 9.23 \text{ g/cm}^3$$

Therefore, its crystal structure is simple cubic.

3.15 The unit cell for tin has tetragonal symmetry, with a and b lattice parameters of 0.583 and 0.318 nm, respectively.   If its density, atomic weight, and atomic radius are 7.30 g/cm^3, 118.69 g/mol, and 0.151 nm, respectively, compute the atomic packing factor.

<u>Solution</u>

In order to determine the APF for Sn, we need to compute both the unit cell volume (V_C) which is just the a^2c product, as well as the total sphere volume (V_S) which is just the product of the volume of a single sphere and the number of spheres in the unit cell (n). The value of n may be calculated from Equation 3.5 as

$$n = \frac{\rho V_C N_A}{A_{Sn}}$$

$$= \frac{(7.30 \text{ g/cm}^3)(5.83)^2(3.18)\left(\times 10^{-24} \text{ cm}^3\right)\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}{118.69 \text{ g/mol}}$$

= 4.00 atoms/unit cell

Therefore

$$\text{APF} = \frac{V_S}{V_C} = \frac{(4)\left(\frac{4}{3}\pi R^3\right)}{(a)^2(c)}$$

$$= \frac{(4)\left[\frac{4}{3}(\pi)(1.51 \times 10^{-8} \text{ cm})^3\right]}{(5.83 \times 10^{-8} \text{ cm})^2(3.18 \times 10^{-8} \text{ cm})}$$

= 0.534

3.16 Iodine has an orthorhombic unit cell for which the a, b, and c lattice parameters are 0.479, 0.725, and 0.978 nm, respectively.

(a) If the atomic packing factor and atomic radius are 0.547 and 0.177 nm, respectively, determine the number of atoms in each unit cell.

(b) 7KHÐWRPLFŽHLJKWÐIŁRGLQHLVŽᴸᴸ̸Ⴤ ̸ᴶĴP RO̸FRP SXWHᵗWKHᵗKHRUHᵗᴶFDОGHQVLWᵗᴸ

Solution

(a) For indium, and from the definition of the APF

$$ APF \; = \; \frac{V_S}{V_C} \; = \; \frac{n\left(\dfrac{4}{3}\pi R^3\right)}{abc} $$

we may solve for the number of atoms per unit cell, n, as

$$ n \; = \; \frac{(APF)\,abc}{\dfrac{4}{3}\pi R^3} $$

Incorporating values of the above parameters provided in the problem state leads to

$$ = \; \frac{(0.547)(4.79 \; \times \; 10^{-8} \text{ cm})(7.25 \; \times \; 10^{-8} \text{ cm})\left(9.78 \; \times \; 10^{-8} \text{ cm}\right)}{\dfrac{4}{3}\pi\left(1.77 \; \times \; 10^{-8} \text{ cm}\right)^3} $$

$$ = 8.0 \text{ atoms/unit cell} $$

(b) In order to compute the density, we just employ Equation 3.5 as

$$ \rho \; = \; \frac{nA_I}{abc\, N_A} $$

$$ = \; \frac{(8 \text{ atoms/unit cell})(126.91 \text{ g/mol})}{\left\{\left[(4.79 \; \times \; 10^{-8} \text{ cm})(7.25 \; \times \; 10^{-8} \text{ cm})\left(9.78 \; \times \; 10^{-8} \text{ cm}\right)\right]/\text{unit cell}\right\}(6.022 \; \times \; 10^{23} \text{ atoms/mol})} $$

$$ = 4.96 \text{ g/cm}^3 $$

3. 17 Titanium has an HCP unit cell for which the ratio of the lattice parameters c/a is 1.58. If the radius of the Ti atom is 0.1445 nm, (a) determine the unit cell volume, and (b) calculate the density of Ti and compare it with the literature value.

Solution

(a) We are asked to calculate the unit cell volume for Ti. For HCP, from Equation 3.S1 (found in the solution to Problem 3.6)

$$V_C = 6R^2c\sqrt{3}$$

But for Ti, c = 1.58a, and a = 2R, or c = 3.16R, and

$$V_C = (6)(3.16)\ R^3\sqrt{3}$$

$$= (6)\,(3.16)\left(\sqrt{3}\right)\left[1.445\ \times\ 10^{-8}\ cm\right]^3 = 9.91\ \times\ 10^{-23}\ cm^3/unit\ cell$$

(b) The theoretical density of Ti is determined, using Equation 3.5, as follows:

$$\rho = \frac{nA_{Ti}}{V_C N_A}$$

For HCP, n = 6 atoms/unit cell, and for Ti, A_{Ti} = 47.87 g/mol (as noted inside the front cover). Thus,

$$\rho = \frac{(6\ atoms/unit\ cell)(47.87\ g/mol)}{\left(9.91\ \times\ 10^{-23}\ cm^3/unit\ cell\right)\left(6.022\ \times\ 10^{23}\ atoms/mol\right)}$$

$$= 4.81\ g/cm^3$$

The value given in the literature is 4.51 g/cm^3.

3.18 Zinc has an HCP crystal structure, a c/a ratio of 1.856, and a density of 7.13 g/cm^3. Compute the atomic radius for Zn.

Solution

In order to calculate the atomic radius for Zn, we must use Equation 3.5, as well as the expression which relates the atomic radius to the unit cell volume for HCP ﾎ ｴ TXDﾡMﾚRQ ﾡ6ﾡb1URﾡﾗ P ﾡ3UREQﾘP ﾡｭﾟﾘﾑ LﾑﾚV DﾑﾚV Rﾐ OﾐRﾑ ZﾚV

$$V_C = 6R^2 c\sqrt{3}$$

In this case c = 1.856a, but, for HCP, a = 2R, which means that

$$V_C = 6R^2(1.856)(2R)\sqrt{3} = (1.856)(12\sqrt{3})R^3$$

And from Equation 3.5, the density is equal to

$$\rho = \frac{nA_{Zn}}{V_C N_A} = \frac{nA_{Zn}}{(1.856)(12\sqrt{3})R^3 N_A}$$

And, solving for R from the above equation leads to the following:

$$R = \left[\frac{nA_{Zn}}{(1.856)\left(12\sqrt{3}\right)\rho N_A}\right]^{1/3}$$

And incorporating appropriate values for the parameters in this equation leads to

$$R = \left[\frac{(6 \text{ atoms/unit cell}) (65.41 \text{ g/mol})}{(1.856)\left(12\sqrt{3}\right)\left(7.13 \text{ g/cm}^3\right)\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}\right]^{1/3}$$

$$= 1.33 \times 10^{-8} \text{ cm} = 0.133 \text{ nm}$$

3.19   Rhenium has an HCP crystal structure, an atomic radius of 0.137 nm, and a c/a ratio of 1.615. Compute the volume of the unit cell for Re.

<u>Solution</u>

In order to compute the volume of the unit cell for Re, it is necessary to use Equation 3.S1 (found in Problem 3.6), that is

$$V_C = 6R^2c\sqrt{3}$$

The problem states that c = 1.615a, and a = 2R. Therefore

$$V_C = (1.615)\left(12\sqrt{3}\right)R^3$$

$$= (1.615)\left(12\sqrt{3}\right)(1.37 \times 10^{-8} \text{ cm})^3 = 8.63 \times 10^{-23} \text{ cm}^3 = 8.63 \times 10^{-2} \text{ nm}^3$$

Crystal Systems

3.20 Below is a unit cell for a hypothetical metal.

(a) To which crystal system does this unit cell belong?

(b) What would this crystal structure be called?

(c) Calculate the density of the material, given that its atomic weight is 141 g/mol.
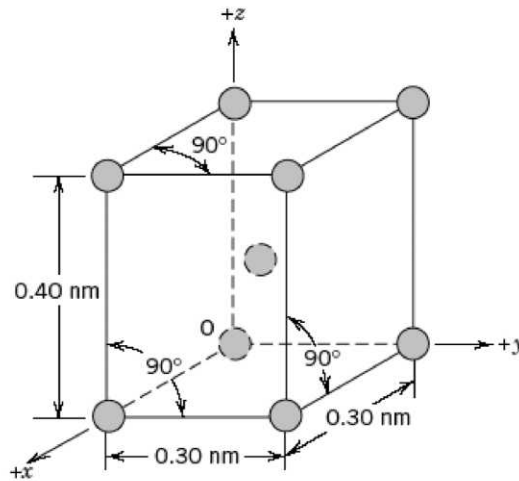
Solution

(a) The unit cell shown in the problem statement belongs to the tetragonal crystal system since a = b = 0.30 nm, c = 0.40 nm, and $\alpha = \beta = \gamma = 90°$.

(b) The crystal structure would be called body-centered tetragonal.

(c) As with BCC, n = 2 atoms/unit cell. Also, for this unit cell

$$V_C = (3.0 \times 10^{-8} \text{ cm})^2 (4.0 \times 10^{-8} \text{ cm})$$

$$= 3.60 \times 10^{-23} \text{ cm}^3/\text{unit cell}$$

Thus, using Equation 3.5, the density is equal to

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

$$= \frac{(2 \text{ atoms/unit cell}) (141 \text{ g/mol})}{(3.60 \times 10^{-23} \text{ cm}^3/\text{unit cell})(6.022 \times 10^{23} \text{ atoms/mol})}$$

$$= 13.0 \text{ g/cm}^3$$

3.21 Sketch a unit cell for the body-centered orthorhombic crystal structure.

Solution

A unit cell for the body-centered orthorhombic crystal structure is presented below.
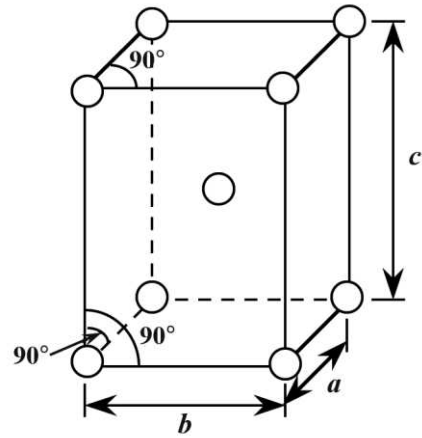
Point Coordinates

3.22 List the point coordinates for all atoms that are associated with the FCC unit cell (Figure 3.1).

<u>Solution</u>

From Figure 3.1b, the atom located of the origin of the unit cell has the coordinates 000. Coordinates for other atoms in the bottom face are 100, 110, 010, and $\frac{1}{2}\frac{1}{2}0$. (The z coordinate for all these points is zero.)

For the top unit cell face, the coordinates are 001, 101, 111, 011, and $\frac{1}{2}\frac{1}{2}1$.

Coordinates for those atoms that are positioned at the centers of both side faces, and centers of both front and back faces need to be specified. For the front and back-center face atoms, the coordinates are $1\frac{1}{2}\frac{1}{2}$ and $0\frac{1}{2}\frac{1}{2}$, respectively. While for the left and right side center-face atoms, the respective coordinates are $\frac{1}{2}0\frac{1}{2}$ and $\frac{1}{2}1\frac{1}{2}$.

3.23 List the point coordinates of the titanium, barium, and oxygen ions for a unit cell of the perovskite crystal structure (Figure 12.6).

Solution

In Figure 12.6, the barium ions are situated at all corner positions. The point coordinates for these ions are as follows: 000, 100, 110, 010, 001, 101, 111, and 011.

The oxygen ions are located at all face-centered positions; therefore, their coordinates are $\frac{1}{2}\frac{1}{2}0$, $\frac{1}{2}\frac{1}{2}1$, $1\frac{1}{2}\frac{1}{2}$, $0\frac{1}{2}\frac{1}{2}$, $\frac{1}{2}0\frac{1}{2}$, and $\frac{1}{2}1\frac{1}{2}$.

And, finally, the titanium ion resides at the center of the cubic unit cell, with coordinates $\frac{1}{2}\frac{1}{2}\frac{1}{2}$.

3.24 List the point coordinates of all atoms that are associated with the diamond cubic unit cell (Figure 12.15).

<u>Solution</u>

First of all, one set of carbon atoms occupy all corner positions of the cubic unit cell; the coordinates of these atoms are as follows: 000, 100, 110, 010, 001, 101, 111, and 011.

Another set of atoms reside on all of the face-centered positions, with the following coordinates: $\frac{1}{2}\frac{1}{2}0$, $\frac{1}{2}\frac{1}{2}1$, $1\frac{1}{2}\frac{1}{2}$, $0\frac{1}{2}\frac{1}{2}$, $\frac{1}{2}0\frac{1}{2}$, and $\frac{1}{2}1\frac{1}{2}$.

The third set of carbon atoms are positioned within the interior of the unit cell. Using an x-y-z coordinate system oriented as in Figure 3.4, the coordinates of the atom that lies toward the lower-left-front of the unit cell has the coordinates $\frac{3}{4}\frac{1}{4}\frac{1}{4}$, whereas the atom situated toward the lower-right-back of the unit cell has coordinates of $\frac{1}{4}\frac{3}{4}\frac{1}{4}$. Also, the carbon atom that resides toward the upper-left-back of the unit cell has the $\frac{1}{4}\frac{1}{4}\frac{3}{4}$ coordinates. And, the coordinates of the final atom, located toward the upper-right-front of the unit cell, are $\frac{3}{4}\frac{3}{4}\frac{3}{4}$.

3.25 Sketch a tetragonal unit cell , and within that cell indicate locations of the $\frac{1}{2}$ 1 $\frac{1}{2}$ and $\frac{1}{4}$ $\frac{1}{2}$ $\frac{3}{4}$ point coordinates.

Solution

A tetragonal unit in which are shown the $\frac{1}{2}$ 1 $\frac{1}{2}$ and $\frac{1}{4}\frac{1}{2}\frac{3}{4}$ point coordinates is presented below.
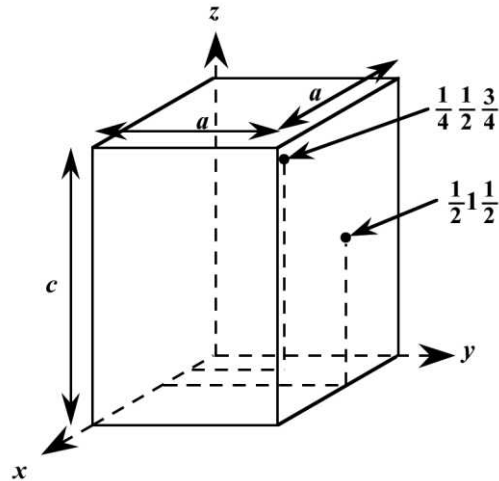
3.26   Using the Molecule Definition Utility found in both "Metallic Crystal Structures and Crystallography" and "Ceramic Crystal Structures" modules of VMSE, located on the book's web site [www.wiley.com/college/Callister (Student Companion Site)], generate a three-dimensional unit cell for the intermetallic compound $AuCu_3$ given the following: (1) the unit cell is cubic with an edge length of 0.374 nm, (2) gold atoms are situated at all cube corners, and (3) copper atoms are positioned at the centers of all unit cell faces.

Solution

First of all, open the "Molecular Definition Utility"; it may be found in either of "Metallic Crystal Structures and Crystallography" or "Ceramic Crystal Structures" modules.

In the "Step 1" window, it is necessary to define the atom types, colors for the spheres (atoms), and specify atom sizes. Let us enter "Au" as the name for the gold atoms (since "Au" the symbol for gold), and "Cu" as the name for the copper atoms. Next it is necessary to choose a color for each atom type from the selections that appear in the pull-down menu—for example, "Yellow" for Au and "Red" for Cu. In the "Atom Size" window, it is necessary to enter an atom/ion size. In the instructions for this step, it is suggested that the atom/ion diameter in nanometers be used. From the table found inside the front cover of the textbook, the atomic radii for gold and copper are 0.144 nm and 0.128 nm, respectively, and, therefore, their ionic diameters are twice these values (i⧨⧨⧨⧨⧨⧨⧨⧨⧨QP ⧨DQG⧨⧨⧨QP♀⧠ therefore, we enter the values "0.288" and "0.256" for the two atom types. Now click on the "Register" button, followed by clicking on the "Go to Step 2" button.

In the "Step 2" window we specify positions for all of the atoms within the unit cell; their point coordinates are specified in the problem statement. Let's begin with gold. Click on the yellow sphere that is located to the right of the "Molecule Definition Utility" box. Again, Au atoms are situated at all eight corners of the cubic unit cell. One Au will be positioned at the origin of the coordinate system—i.e., its point coordinates are 000, and, therefore, we enter a "0" (zero) in each of the "x", "y", and "z" atom position boxes. Next we click on the "Register Atom Position" button. Now we enter the coordinates of another gold atom; let us arbitrarily select the one that resides at the corner of the unit cell that is one unit-cell length along the x-axis (i.e., at the 100 point coordinate). Inasmuch as it is located a distance of a units along the x-axis the value of "0.374" is entered in the "x" atom position box (since this is the value of a given in the problem statement); zeros are entered in each of the "y" and "z" position boxes. We repeat this procedure for the remaining six Au atoms.

After this step has been completed, it is necessary to specify positions for the copper atoms, which are located at all six face-centered sites. To begin, we click on the red sphere that is located next to the "Molecule Definition Utility" box. The point coordinates for some of the Cu atoms are fractional ones; in these instances, the a unit cell length (i.e., 0.374) is multiplied by the fraction. For example, one Cu atom is located $1\frac{1}{2}\frac{1}{2}$ coordinate. Therefore, the x, y, and z atoms positions are (1)(0.374) = 0.374, $\frac{1}{2}(0.374) = 0.187$, and $\frac{1}{2}(0.374) = 0.187$, respectively.

For the gold atoms, the x, y, and z atom position entries for all 8 sets of point coordinates are as follows:

0, 0, and 0

0.374, 0, and 0

0, 0.374, and 0

0, 0, and 0.374

0, 0.374, 0.374

0.374, 0, 0.374

0.374, 0.374, 0

0.374, 0.374, 0.374

Now, for the copper atoms, the x, y, and z atom position entries for all 6 sets of point coordinates are as follows:

0.187, 0.187, 0

0.187, 0, 0.187

0, 0.187, 0.187

0.374, 0.187, 0.187

0.187, 0.374, 0.187

0.187, 0.187, 0.374

In Step 3, we may specify which atoms are to be represented as being bonded to one another, and which type of bond(s) to use (single solid, single dashed, double, and triple are possibilities), or we may elect to not represent any bonds at all (in which case we are finished). If it is decided to show bonds, probably the best thing to do is to represent unit cell edges as bonds. This image may be rotated by using mouse click-and-drag

Your image should appear as the following screen shot. Here the gold atoms appear lighter than the copper atoms.
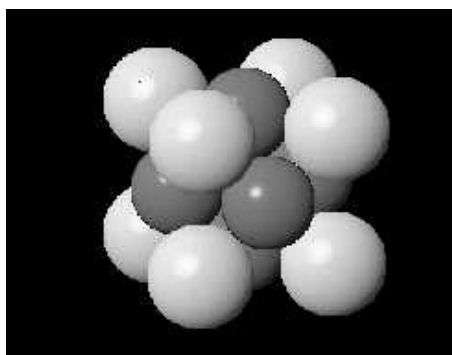
[Note: Unfortunately, with this version of the Molecular Definition Utility, it is not possible to save either the data or the image that you have generated. You may use screen capture (or screen shot) software to record and store your image.]

Crystallographic Directions

3.27 Draw an orthorhombic unit cell, and within that cell a $[12\bar{1}]$ direction.

<u>Solution</u>

This problem calls for us to draw a $[12\bar{1}]$ direction within an orthorhombic unit cell (a ≠ b ≠ c, α = β = γ = 90°). Such a unit cell with its origin positioned at point O is shown below. We first move along the +x-axis a units (from point O to point A), then parallel to the +y-axis 2b units (from point A to point B). Finally, we proceed parallel to the z-axis -c units (from point B to point C). The $[12\bar{1}]$ direction is the vector from the origin (point O) to point C as shown.
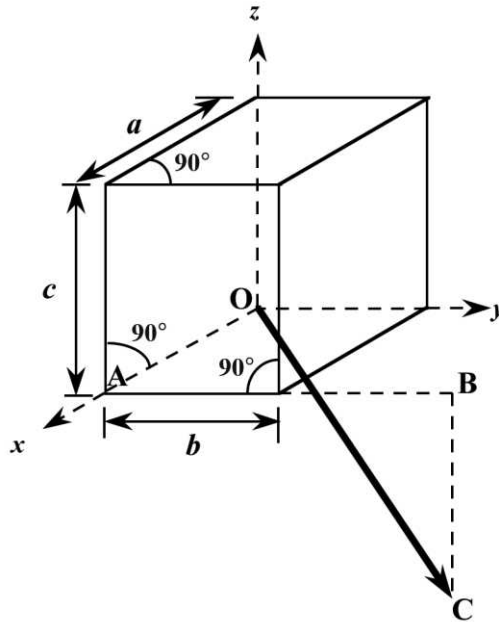
3.28 Sketch a monoclinic unit cell, and within that cell a $[0\bar{1}1]$ direction.

Solution

This problem asks that a $[0\bar{1}1]$ direction be drawn within a monoclinic unit cell (a ≠ b ≠ c, and α = β = 90° ≠ γ). One such unit cell with its origin at point O is sketched below. For this direction, there is no projection along the x-axis since the first index is zero; thus, the direction lies in the y-z plane. We next move from the origin along the minus y-axis b units (from point O to point R). Since the final index is a one, move from point R parallel to the z-axis, c units (to point P). Thus, the $[0\bar{1}1]$ direction corresponds to the vector passing from the origin (point O) to point P, as indicated in the figure.
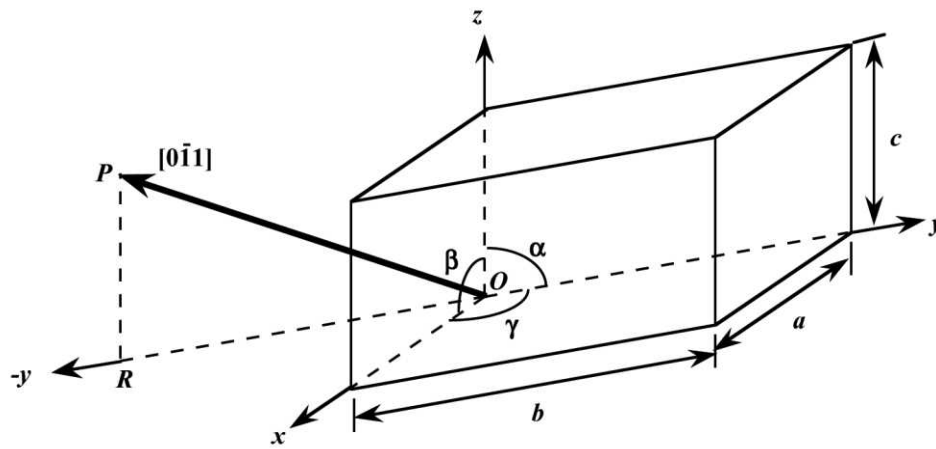
3.29 What are the indices for the directions indicated by the two vectors in the sketch below?
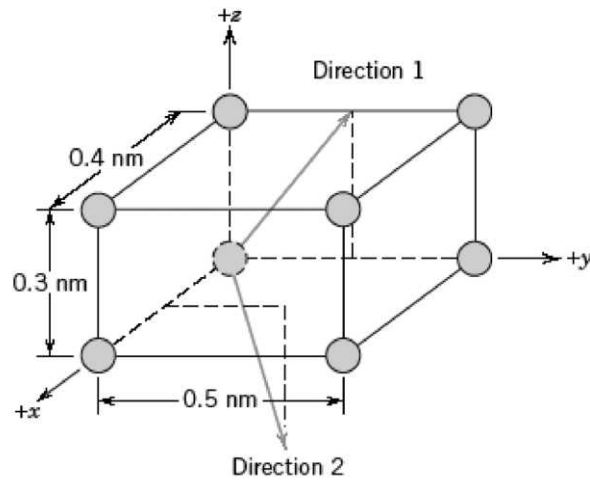
Solution

For direction 1, the projection on the x-axis is zero (since it lies in the y-z plane), while projections on the y- and z-axes, b/2 and c, respectively. This is a $[012]$ direction as indicated in the summary below.

	x	y	z
Projections	0a	b/2	c
Projections in terms of a, b, and c	0	1/2	1
Reduction to integers	0	1	2
Enclosure		$[012]$	

Direction 2 is $[11\bar{2}]$ as summarized below.

	x	y	z
Projections	a/2	b/2	-c
Projections in terms of a, b, and c	1/2	1/2	-1
Reduction to integers	1	1	-2
Enclosure		$[11\bar{2}]$	

3.30 Within a cubic unit cell, sketch the following directions:

(a) $[\bar{1}10]$,   (e) $[\bar{1}\,\bar{1}\,1]$,

(b) $[\bar{1}\,\bar{2}\,1]$,   (f) $[\bar{1}22]$,

(c) $[0\bar{1}2]$,   (g) $[1\bar{2}\,\bar{3}]$,

(d) $[1\bar{3}3]$,   (h) $[\bar{1}03]$.

<u>Solution</u>

The directions asked for are indicated in the cubic unit cells shown below.
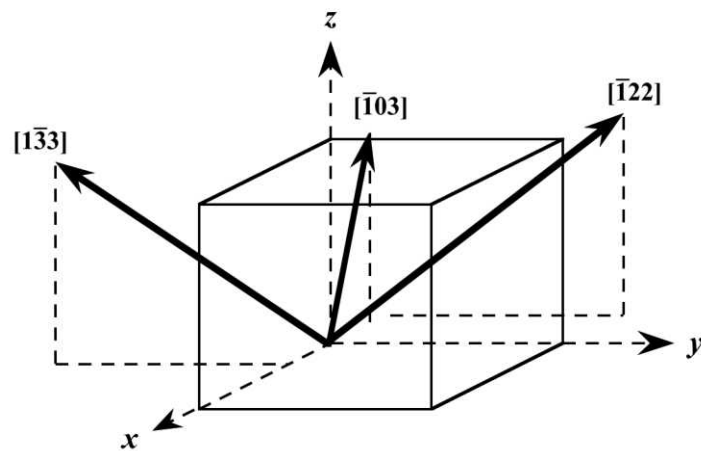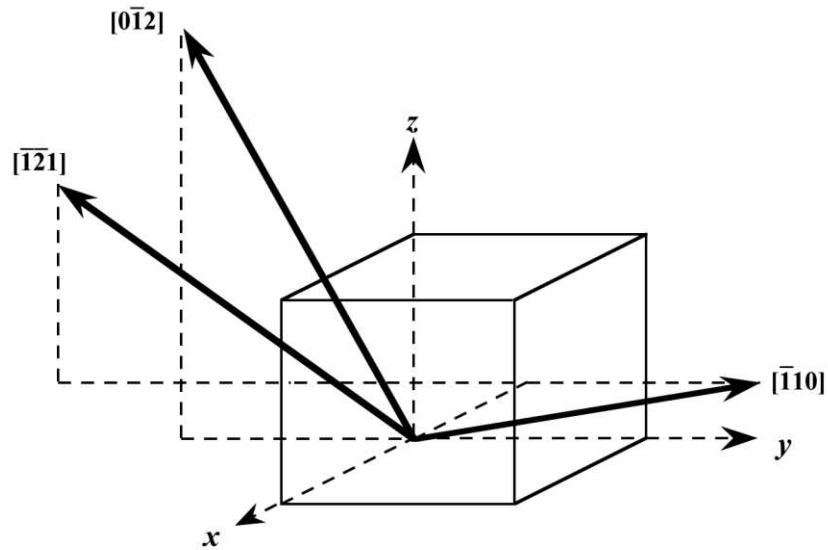
3.31 Determine the indices for the directions shown in the following cubic unit cell:
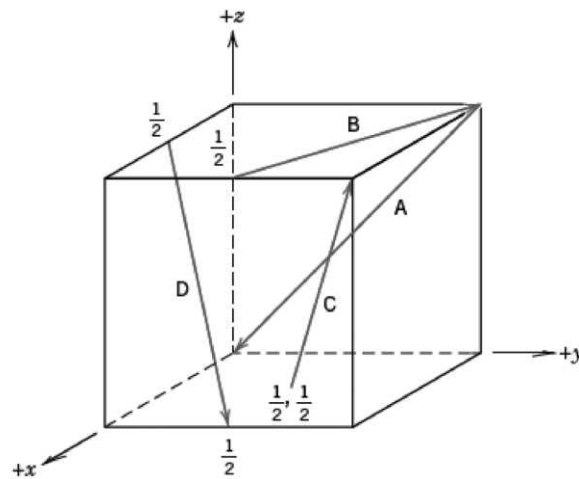
Solution

Direction A is a $[0\bar{1}\,\bar{1}]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	$\underline{x}$	$\underline{y}$	$\underline{z}$
Projections	0a	−b	−c
Projections in terms of a, b, and c	0	−1	−1
Reduction to integers		not necessary	
Enclosure		$[0\bar{1}\,\bar{1}]$	

Direction B is a $[\bar{2}10]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	$\underline{x}$	$\underline{y}$	$\underline{z}$
Projections	−a	$\dfrac{b}{2}$	0c
Projections in terms of a, b, and c	−1	$\dfrac{1}{2}$	0
Reduction to integers	−2	1	0
Enclosure		$[\bar{2}10]$	

Direction C is a [112] direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	x	y	z
Projections	$\dfrac{a}{2}$	$\dfrac{b}{2}$	c
Projections in terms of a, b, and c	$\dfrac{1}{2}$	$\dfrac{1}{2}$	1
Reduction to integers	1	1	2
Enclosure		[112]	

Direction D is a $[11\bar{2}]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	x	y	z
Projections	$\dfrac{a}{2}$	$\dfrac{b}{2}$	−c
Projections in terms of a, b, and c	$\dfrac{1}{2}$	$\dfrac{1}{2}$	−1
Reduction to integers	1	1	−2
Enclosure		$[11\bar{2}]$	

3.32 Determine the indices for the directions shown in the following cubic unit cell:
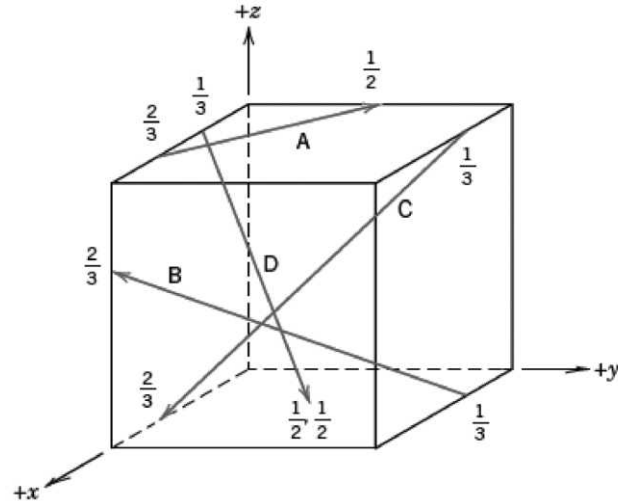
Solution

Direction A is a $[\bar{4}30]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	x	y	z
Projections	$-\dfrac{2a}{3}$	$\dfrac{b}{2}$	0c
Projections in terms of a, b, and c	$-\dfrac{2}{3}$	$\dfrac{1}{2}$	0
Reduction to integers	–4	3	0
Enclosure		$[\bar{4}30]$	

Direction B is a $[2\bar{3}2]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	x	y	z
Projections	$\dfrac{2a}{3}$	$-b$	$\dfrac{2c}{3}$
Projections in terms of a, b, and c	$\dfrac{2}{3}$	-1	$\dfrac{2}{3}$
Reduction to integers	2	–3	2
Enclosure		$[2\bar{3}2]$	

Direction C is a $[1\bar{3}\bar{3}]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	x	y	z
Projections	$\dfrac{a}{3}$	−b	−c
Projections in terms of a, b, and c	$\dfrac{1}{3}$	−1	−1
Reduction to integers	1	−3	−3
Enclosure		$[1\bar{3}\bar{3}]$	

Direction D is a $[13\bar{6}]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	x	y	z
Projections	$\dfrac{a}{6}$	$\dfrac{b}{2}$	−c
Projections in terms of a, b, and c	$\dfrac{1}{6}$	$\dfrac{1}{2}$	−1
Reduction to integers	1	3	−6
Enclosure		$[13\bar{6}]$	

3.33 For tetragonal crystals, cite the indices of directions that are equivalent to each of the following directions:

(a) [001]

(b) [110]

(c) [010]

Solution

For tetragonal crystals $a = b \neq c$ and $\alpha = \beta = \gamma = 90°$; therefore, projections along the x and y axes are equivalent, which are not equivalent to projections along the z axis.

(a) Therefore, for the [001] direction, there is only one equivalent direction: $[00\bar{1}]$.

(b) For the [110] direction, equivalent directions are as follows: $[\bar{1}\bar{1}0]$, $[\bar{1}10]$, and $[1\bar{1}0]$

(b) Also, for the [010] direction, equivalent directions are the following: $[0\bar{1}0]$, $[100]$, and $[\bar{1}00]$.

3.34 Convert the [100] and [111] directions into the four-index Miller–Bravais scheme for hexagonal unit cells.

<u>Solution</u>

For [100]

u' = 1,
v' = 0,
w' = 0

From Equations 3.6

$$u = \frac{1}{3}(2u' - v') = \frac{1}{3}[(2)(1) - 0] = \frac{2}{3}$$

$$v = \frac{1}{3}(2v' - u') = \frac{1}{3}[(2)(0) - 1] = -\frac{1}{3}$$

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

$$w = w' = 0$$

It is necessary to multiply these numbers by 3 in order to reduce them to the lowest set of integers. Thus, the direction is represented as $[uvtw] = [2\bar{1}\bar{1}0]$.

For [111], u' = 1, v' = 1, and w' = 1. Therefore,

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

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

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

$$w = 1$$

If we again multiply these numbers by 3, then u = 1, v = 1, t = -2, and w = 3. Thus, the direction is represented as
Thus, the direction is represented as $[uvtw] = [11\bar{2}3]$.

3.35 Determine indices for the directions shown in the following hexagonal unit cells:

Solution
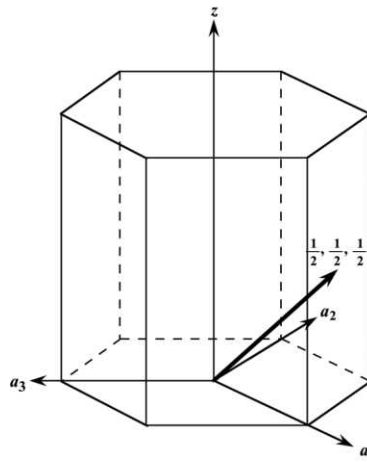
(a)

(a) For this direction, projections on the a_1, a_2, and z axes are a, a/2, and c/2, or, in terms of a and c the projections are 1, 1/2, and 1/2, which when multiplied by the factor 2 become the smallest set of integers: 2, 1, and 1. This means that

u' = 2

v' = 1

w' = 1
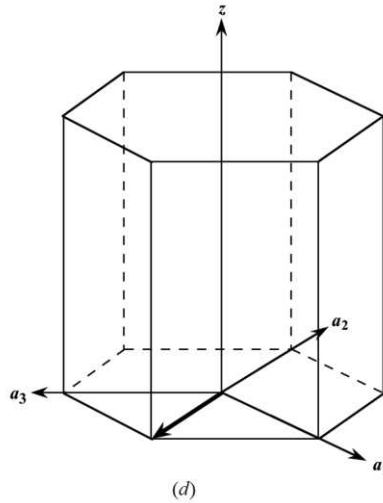
Now, from Equations 3.6, the u, v, t, and w indices become

$$u = \frac{1}{3}(2u' - v') = \frac{1}{3}[(2)(2) - (1)] = \frac{3}{3} = 1$$

$$v = \frac{1}{3}(2v' - u') = \frac{1}{3}[(2)(1) - (2)] = 0$$

$$t = -(u + v) = -(1 + 0) = -1$$

w = w' = 1

No reduction is necessary inasmuch as all of these indices are integers; therefore, this direction in the four-index scheme is $[10\bar{1}1]$

(b)
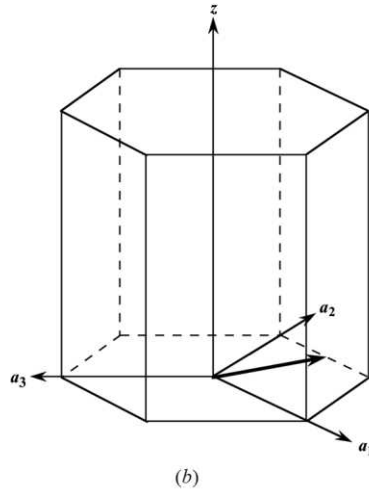
(b) For this direction, projections on the a_1, a_2, and z axes are a/2, a, and 0c, or, in terms of a and c the projections are 1/2, 1, and 0, which when multiplied by the factor 2 become the smallest set of integers: 1, 2, and 0 This means that

$$u' = 1$$
$$v' = 2$$
$$w' = 0$$

Now, from Equations 3.6, the u, v, t, and w indices become

$$u = \frac{1}{3}(2u' - v) = \frac{1}{3}[(2)(1) - 2] = 0$$

$$v = \frac{1}{3}(2v' - u') = \frac{1}{3}[(2)(2) - 1] = 1$$

$$t = -(u+v) = -(0+1) = -1$$

$$w = w' = 0$$

No reduction is necessary inasmuch as all of these indices are integers; therefore, this direction in the four-index scheme is $[01\bar{1}0]$.

(c)
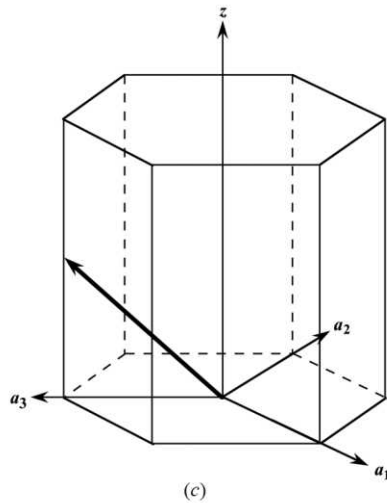
(c) For this direction projections on the a_1, a_2, and z axes are −a, −a, and c/2, or, in terms of a and c the projections are −1, −1, and 1/2, which when multiplied by the factor 2 become the smallest set of integers: −2, −2, and 1. This means that

$$u' = -2$$
$$v' = -2$$
$$w' = 1$$

Now, from Equations 3.6, the u, v, t, and w indices become

$$u = \frac{1}{3}(2u' - v) = \frac{1}{3}[(2)(-2) - (-2)] = -\frac{2}{3}$$

$$v = \frac{1}{3}(2v' - u') = \frac{1}{3}[(2)(-2) - (-2)] = -\frac{2}{3}$$

$$t = -(u + v) = -\left(-\frac{2}{3} - \frac{2}{3}\right) = \frac{4}{3}$$

$$w = w' = 1$$

Now, in order to get the lowest set of integers, it is necessary to multiply all indices by the factor 3, with the result that this direction is a $[\bar{2}\bar{2}43]$ direction.

(d)

(d) For this direction, projections on the a_1, a_2, and z axes are 0a, −a, and 0c, or, in terms of a and c the projections are 0, -1, and 0. This means that

$$u' = 0$$

$$v' = -1$$

$$w' = 0$$

Now, from Equations 3.6, the u, v, t, and w indices become

$$u = \frac{1}{3}(2u' - v') = \frac{1}{3}[(2)(0) - (-1)] = \frac{1}{3}$$

$$v = \frac{1}{3}(2v' - u') = \frac{1}{3}[(2)(-1) - 0] = -\frac{2}{3}$$

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

$$w = w' = 0$$

Now, in order to get the lowest set of integers, it is necessary to multiply all indices by the factor 3, with the result that this is a $[1\bar{2}10]$ direction.

3.36 Sketch the $[\bar{1}\,\bar{1}23]$ and $[10\bar{1}0]$ directions in a hexagonal unit cell.

<u>Solution</u>

The first portion of this problem asks that we plot the $[\bar{1}\,\bar{1}23]$ within a hexagonal unit cell. Below is shown this direction plotted within a hexagonal unit cell having a reduced-scale coordinate scheme.
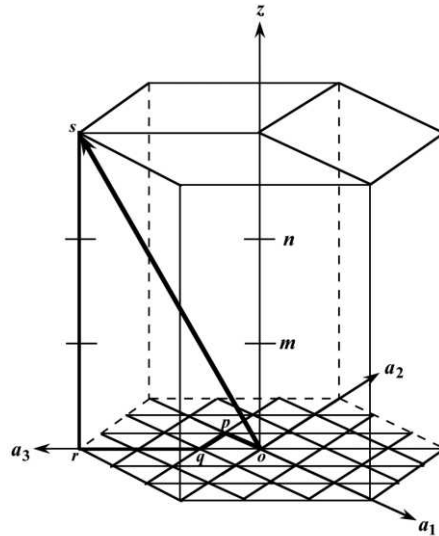
For this direction, projections on the a_1, a_2, a_3, and c axes are respectively, $-1, -1, 2,$ and 3, respectively. In plotting this direction, we begin at the origin of the coordinate system, point o. From here we proceed 1 unit distance along the $-a_1$ axis (to point p), from here 1 unit distance parallel to $-a_2$ axis (to point q), then 2 unit distances parallel (or along) the a_3 axis (to point r), and finally, 3 unit distances parallel to the z axis (to point s). Thus, the $[\bar{1}\,\bar{1}23]$ direction is that vector that extends from point o to point s as shown.

Now we are asked to plot the $[10\bar{1}0]$ within a hexagonal unit cell. In the figure below is plotted this direction within a hexagonal unit cell having a reduced-scale coordinate scheme.
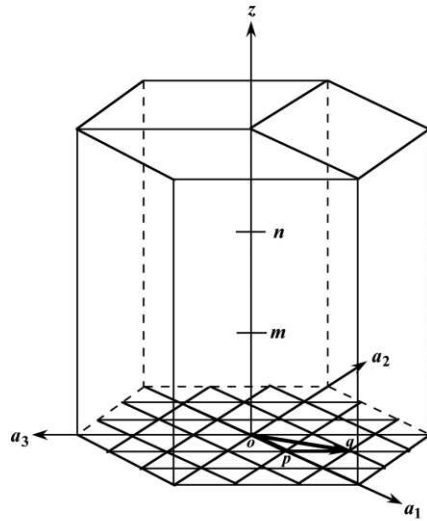
For this direction, projections on the a_1, a_2, a_3, and c axes are respectively, 1, 0, −1, and 0, respectively. In plotting this direction, we begin at the origin of the coordinate system, point o. From here we proceed 1 unit distance along the a_1 axis (to point p). Since there is no projection on the a_2 axis it is not necessary to move parallel to this axis. Therefore, from point p we proceed 1 unit distance parallel to −a_3 axis (to point q). And, finally, inasmuch as there is no projection along the z axis, it is not necessary to move parallel to this axis. Thus, the [10$\bar{1}$0] direction is that vector that extends from point o to point q as shown.

3.37 Using Equations 3.6a, 3.6b, 3.6c, and 3.6d, derive expressions for each of the three primed indices set (u', v', and w') in terms of the four unprimed indices (u, v, t, and w).

<u>Solution</u>

It is first necessary to do an expansion of Equation 3.6a as

$$u = \frac{1}{3}(2u' - v) = \frac{2u'}{3} - \frac{v'}{3}$$

And solving this expression for v' yields

$$v' = 2u' - 3u$$

Now, substitution of this expression into Equation 3.6b gives

$$v = \frac{1}{3}(2v' - u') = \frac{1}{3}[(2)(2u' - 3u) - u'] = u' - 2u$$

Or

$$u' = v + 2u$$

And, solving for v from Equation 3.6c leads to

$$v = -(u + t)$$

which, when substituted into the above expression for u' yields

$$u' = v + 2u = -u - t + 2u = u - t$$

In solving for an expression for v', we begin with the one of the above expressions for this parameter—i.e.,

$$v' = 2u' - 3u$$

Now, substitution of the above expression for u' into this equation leads to

$$v' = 2u' - 3u = (2)(u - t) - 3u = -u - 2t$$

And solving for u from Equation 3.6c gives

$$u = -v - t$$

which, when substituted in the previous equation results in the following expression for v'

$$v' = -u - 2t = -(-v - t) - 2t = v - t$$

And, of course from Equation 3.6d

$$w' = w$$

Crystallographic Planes

3.38 (a) Draw an orthorhombic unit cell, and within that cell a (210) plane.

(b) Draw a monoclinic unit cell, and within that cell a (002) plane.

Solution

(a) We are asked to draw a (210) plane within an orthorhombic unit cell. First remove the three indices from the parentheses, and take their reciprocals--i.e., 1/2, 1, and ∞. This means that the plane intercepts the x-axis at a/2, the y-axis at b, and parallels the z-axis. The plane that satisfies these requirements has been drawn within the orthorhombic unit cell below. (For orthorhombic, $a \neq b \neq c$, and $\alpha = \beta = \gamma = 90°$.)
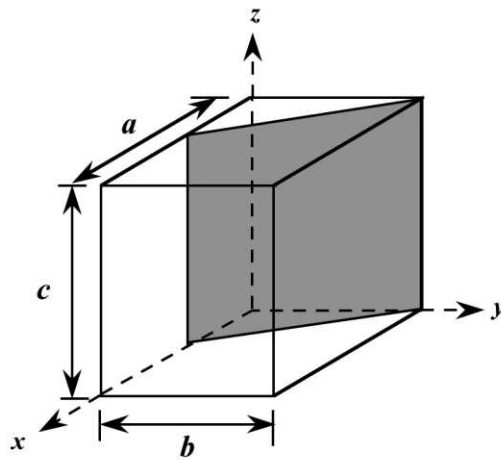
(b) A (002) plane is drawn within the monoclinic cell shown below. We first remove the parentheses and take the reciprocals of the indices; this gives ∞, ∞, and 1/2. Thus, the (002) plane parallels both x- and y-axes, and intercepts the z-axis at a/2, as indicated in the drawing. (For monoclinic, $a \neq b \neq c$, and $\alpha = \gamma = 90° \neq \beta$.)
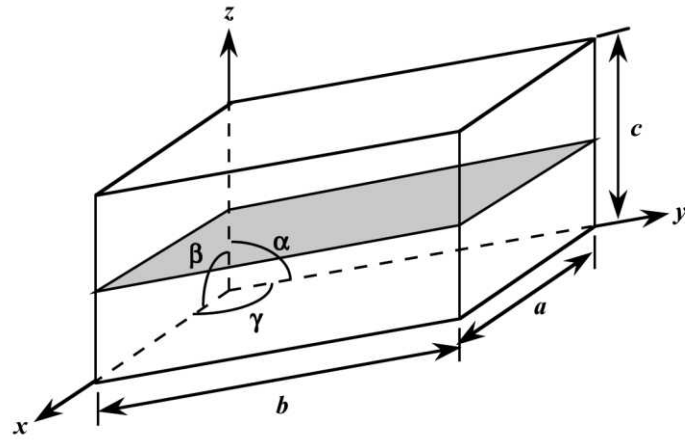
3.39 What are the indices for the two planes drawn in the sketch below?
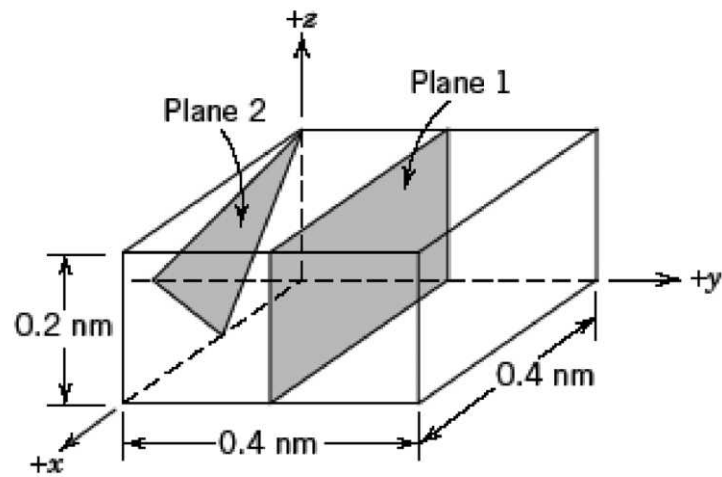
Solution

Plane 1 is a (020) plane. The determination of its indices is summarized below.

	x	y	z
Intercepts	∞a	b/2	∞c
Intercepts in terms of a, b, and c	∞	1/2	∞
Reciprocals of intercepts	0	2	0
Enclosure		(020)	

Plane 2 is a $(2\bar{2}1)$ plane, as summarized below.

	x	y	z
Intercepts	a/2	-b/2	c
Intercepts in terms of a, b, and c	1/2	-1/2	1
Reciprocals of intercepts	2	-2	1
Enclosure		$(2\bar{2}1)$	

3.40 Sketch within a cubic unit cell the following planes:

(a) $(0\bar{1}\bar{1})$,   (e) $(\bar{1}1\bar{1})$,

(b) $(11\bar{2})$,   (f) $(1\bar{2}\bar{2})$,

(c) $(10\bar{2})$,   (g) $(\bar{1}2\bar{3})$,

(d) $(1\bar{3}1)$,   (h) $(0\bar{1}3)$

Solution

The planes called for are plotted in the cubic unit cells shown below.
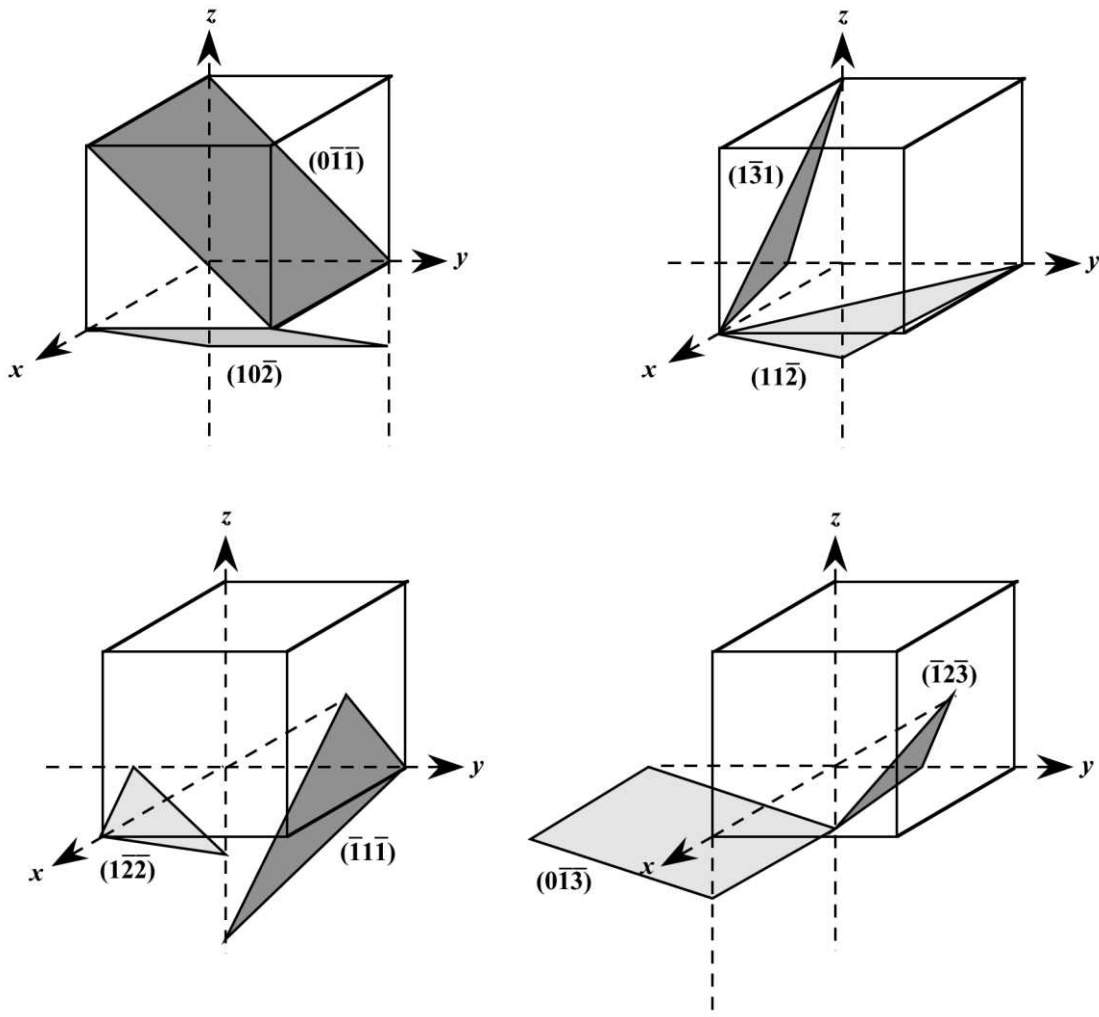
3.41 Determine the Miller indices for the planes shown in the following unit cell:
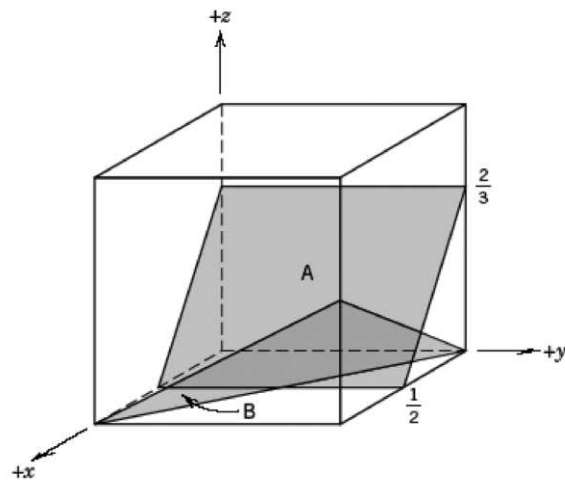
Solution

For plane A we will leave the origin at the unit cell as shown; this is a (403) plane, as summarized below.

	x	y	z
Intercepts	$\dfrac{a}{2}$	∞b	$\dfrac{2c}{3}$
Intercepts in terms of a, b, and c	$\dfrac{1}{2}$	∞	$\dfrac{2}{3}$
Reciprocals of intercepts	2	0	$\dfrac{3}{2}$
Reduction	4	0	3
Enclosure		(403)	

For plane B we will move the origin of the unit cell one unit cell distance to the right along the y axis, and one unit cell distance parallel to the x axis; thus, this is a $(\bar{1}\,\bar{1}2)$ plane, as summarized below.

	x	y	z
Intercepts	$-a$	$-b$	$\dfrac{c}{2}$
Intercepts in terms of a, b, and c	-1	-1	$\dfrac{1}{2}$
Reciprocals of intercepts	-1	-1	2
Reduction		(not necessary)	
Enclosure		$(\bar{1}\,\bar{1}2)$	

3.42 Determine the Miller indices for the planes shown in the following unit cell:

For plane A we will move the origin of the coordinate system one unit cell distance to the upward along the z axis; thus, this is a $(32\bar{2})$ plane, as summarized below.

	x	y	z
Intercepts	$\dfrac{a}{3}$	$\dfrac{b}{2}$	$-\dfrac{c}{2}$
Intercepts in terms of a, b, and c	$\dfrac{1}{3}$	$\dfrac{1}{2}$	$-\dfrac{1}{2}$
Reciprocals of intercepts	3	2	-2
Reduction		(not necessary)	
Enclosure		$(32\bar{2})$	

For plane B we will move the original of the coordinate system on unit cell distance along the x axis; thus, this is a $(\bar{1}01)$ plane, as summarized below.

	x	y	z
Intercepts	$-\dfrac{a}{2}$	∞b	$\dfrac{c}{2}$
Intercepts in terms of a, b, and c	$-\dfrac{1}{2}$	∞	$\dfrac{1}{2}$
Reciprocals of intercepts	-2	0	2
Reduction	-1	0	1
Enclosure		$(\bar{1}01)$	

3.43 Determine the Miller indices for the planes shown in the following unit cell:
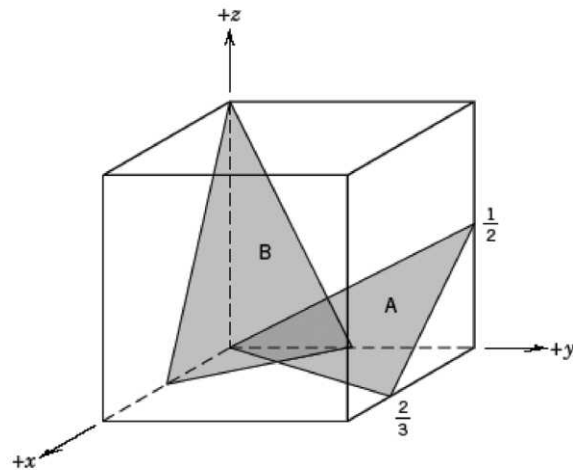
Solution

For plane A since the plane passes through the origin of the coordinate system as shown, we will move the origin of the coordinate system one unit cell distance to the right along the y axis; thus, this is a $(3\bar{2}4)$ plane, as summarized below.

	x	y	z
Intercepts	$\dfrac{2a}{3}$	$-b$	$\dfrac{c}{2}$
Intercepts in terms of a, b, and c	$\dfrac{2}{3}$	-1	$\dfrac{1}{2}$
Reciprocals of intercepts	$\dfrac{3}{2}$	-1	2
Reduction	3	-2	4
Enclosure		$(3\bar{2}4)$	

For plane B we will leave the origin at the unit cell as shown, this is a (221) plane, as summarized below.

	x	y	z
Intercepts	$\dfrac{a}{2}$	$\dfrac{b}{2}$	c
Intercepts in terms of a, b, and c	$\dfrac{1}{2}$	$\dfrac{1}{2}$	1
Reciprocals of intercepts	2	2	1
Reduction		not necessary	
Enclosure		(221)	

3.44 Cite the indices of the direction that results from the intersection of each of the following pair of planes within a cubic crystal: (a) (100) and (010) planes, (b) (111) and (11$\bar{1}$) planes, and (c) (10$\bar{1}$) and (001) planes.

<u>Solution</u>

(a) In the figure below is shown (100) and (010) planes, and, as indicated, their intersection results in a [001], or equivalently, a [00$\bar{1}$] direction.
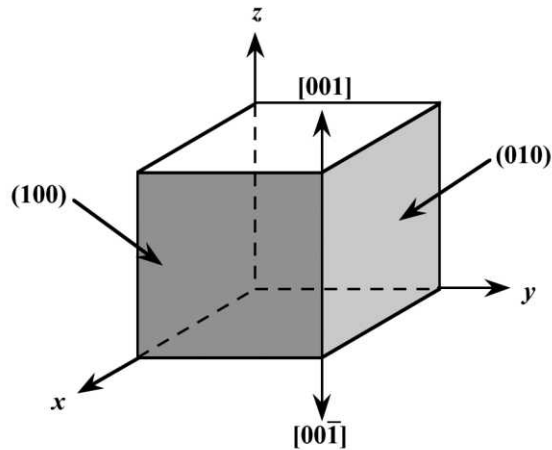

(b) In the figure below is shown (111) and (11$\bar{1}$) planes, and, as indicated, their intersection results in a [$\bar{1}$10], or equivalently, a [1$\bar{1}$0] direction.
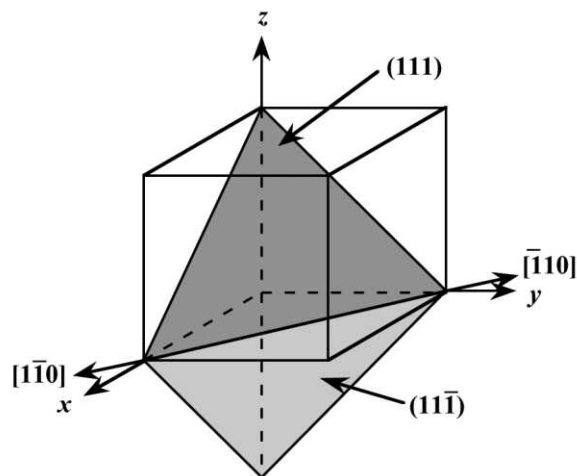
(c) In the figure below is shown $(10\bar{1})$ and (001) planes, and, as indicated, their intersection results in a [010], or equivalently, a $[0\bar{1}0]$ direction.
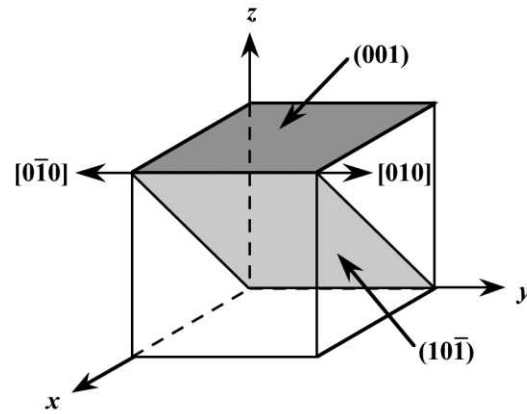
3.45 Sketch the atomic packing of (a) the (100) plane for the BCC crystal structure, and (b) the (201) plane for the FCC crystal structure (similar to Figures 3.10b and 3.11b).

Solution

(a) A BCC unit cell, its (100) plane, and the atomic packing of this plane are indicated below. Corresponding atom positions in the two drawings are indicated by letters W, X, Y, and Z.
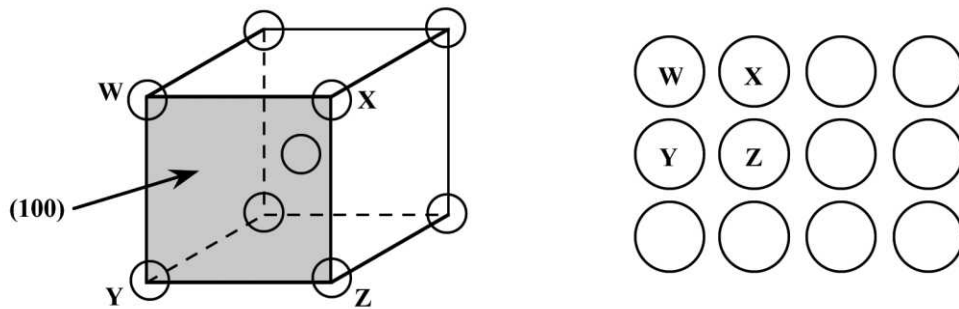
(b) An FCC unit cell, its (201) plane, and the atomic packing of this plane are indicated below. Corresponding atom positions in the two drawing are indicated by the letters A, B, and C.
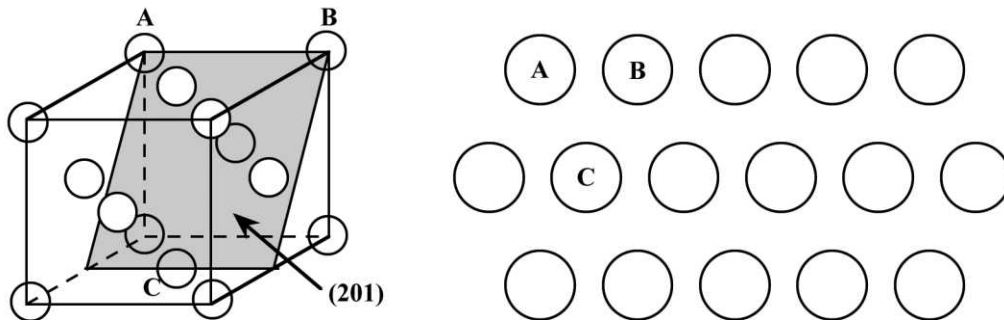
3.46 Consider the reduced-sphere unit cell shown in Problem 3.20, having an origin of the coordinate system positioned at the atom labeled with an O. For the following sets of planes, determine which are equivalent:

(a) $(00\bar{1})$, (010), and, $(\bar{1}00)$

(b) $(1\bar{1}0)$, $(10\bar{1})$, $(0\bar{1}1)$, and $(\bar{1}\bar{1}0)$

(c) $(\bar{1}\bar{1}\bar{1})$, $(\bar{1}1\bar{1})$, $(\bar{1}\bar{1}1)$, and $(1\bar{1}1)$
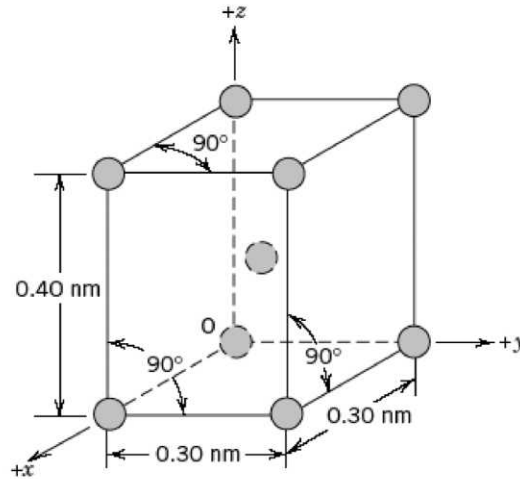
Solution

(a) The unit cell in Problem 3.20 is body-centered tetragonal. Of the three planes given in the problem statement the $(\bar{1}00)$ and (010) are equivalent—that is, have the same atomic packing. The atomic packing for these two planes as well as the $(00\bar{1})$ are shown in the figure below.

$(\bar{1}00)$, (010)

$(00\bar{1})$
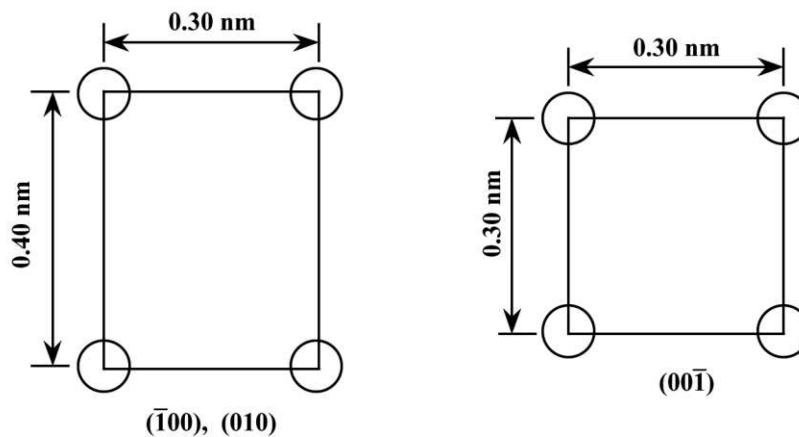
(b) Of the four planes cited in the problem statement, $(1\bar{1}0)$ and $(\bar{1}\bar{1}0)$ are equivalent to one another— have the same atomic packing. The atomic arrangement of these planes is shown in the left drawing below.

Furthermore, the $(10\bar{1})$ and $(0\bar{1}1)$ are equivalent to each other (but not to the other pair of planes); their atomic arrangement is represented in the other drawing. Note: the 0.424 nm dimension in the left-most drawing comes from the relationship $\left[(0.30\,\text{nm})^2 + (0.30\,\text{nm})^2\right]^{1/2}$. Likewise, the 0.500 nm dimension found in the right-most drawing comes from $\left[(0.30\,\text{nm})^2 + (0.40\,\text{nm})^2\right]^{1/2}$.

$(1\bar{1}0), (\bar{1}\bar{1}0)$

$(10\bar{1}), (0\bar{1}1)$
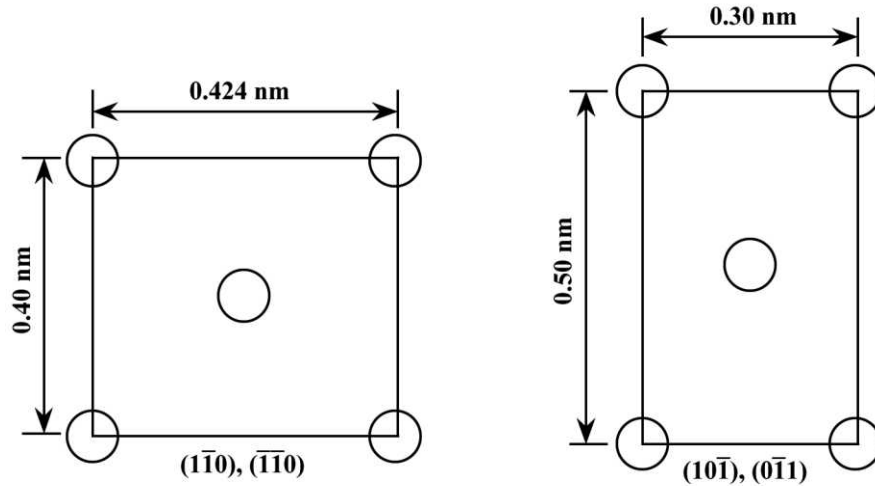
    (c) All of the $(\bar{1}\bar{1}\bar{1})$, $(\bar{1}1\bar{1})$, $(\bar{1}\bar{1}1)$, and $(1\bar{1}1)$ planes are equivalent, that is, have the same atomic packing as illustrated in the following figure:
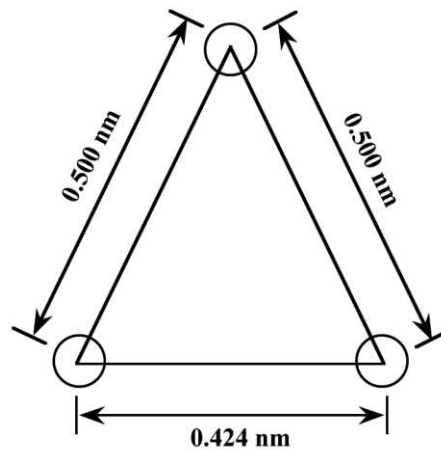
3.47 Here are shown the atomic packing schemes for several different crystallographic directions for some hypothetical metal. For each direction the circles represent only those atoms contained within a unit cell, which circles are reduced from their actual size.
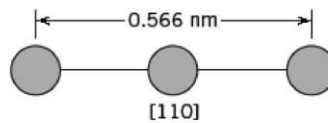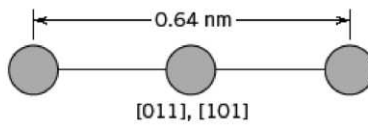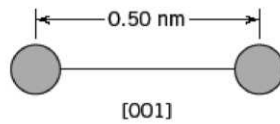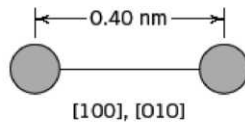
[100], [010]

[001]

[011], [101]

[110]

(a) To what crystal system does the unit cell belong?
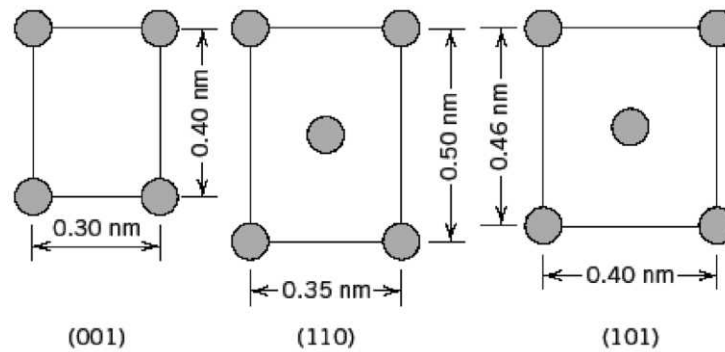
(b) What would this crystal structure be called?

Solution

Below is constructed a unit cell using the six crystallographic directions that were provided in the problem.
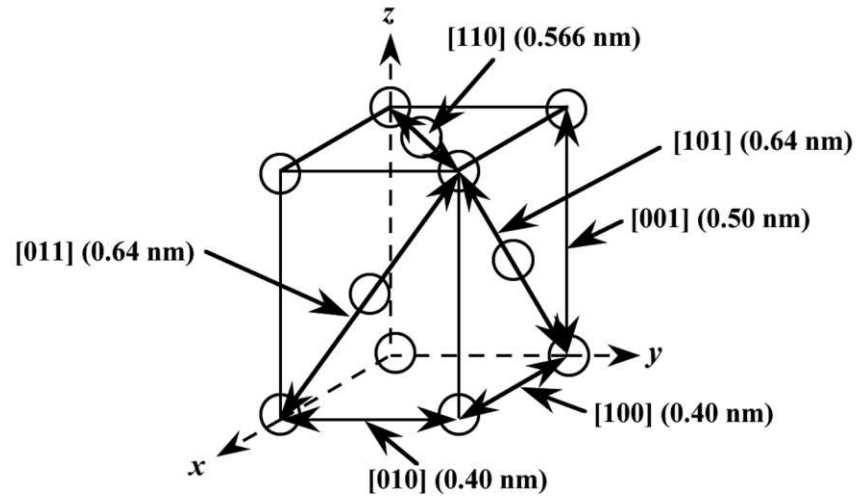
(a) This unit cell belongs to the tetragonal system since a = b = 0.40 nm, c = 0.50 nm, and α = β = γ = 90°.

(b) This crystal structure would be called face-centered tetragonal since the unit cell has tetragonal symmetry, and an atom is located at each of the corners, as well as at the centers of all six unit cell faces. In the figure above, atoms are only shown at the centers of three faces; however, atoms would also be situated at opposite faces.

3.48 Below are shown three different crystallographic planes for a unit cell of some hypothetical metal. The circles represent atoms:

(001)   (110)   (101)

(a) To what crystal system does the unit cell belong?

(b) What would this crystal structure be called?

(c) If the density of this metal is 8.95 g/cm^3, determine its atomic weight.

Solution

The unit cells constructed below show the three crystallographic planes that were provided in the problem statement.
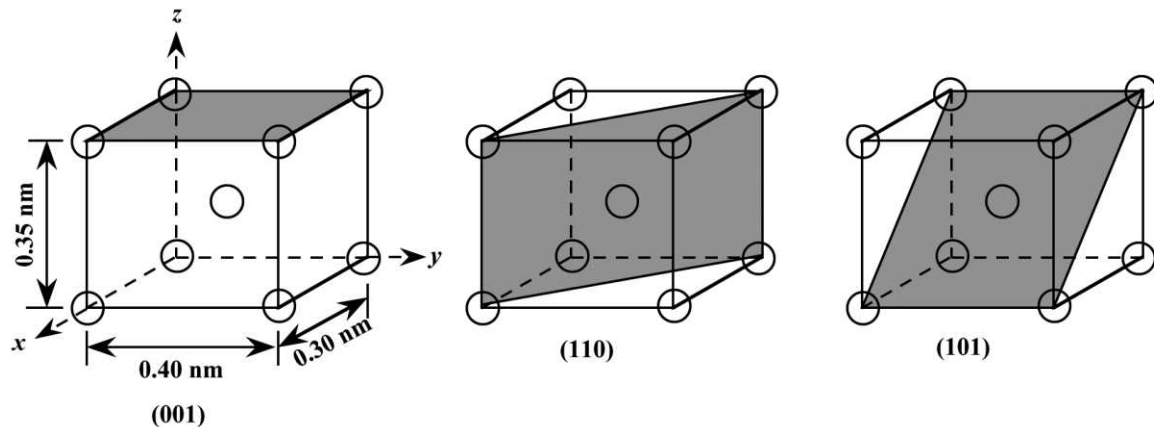
(a) This unit cell belongs to the orthorhombic crystal system since a = 0.30 nm, b = 0.40 nm, c = 0.35 nm, and α = β = γ = 90°.

(b) This crystal structure would be called body-centered orthorhombic since the unit cell has orthorhombic symmetry, and an atom is located at each of the corners, as well as at the cell center.

(c) In order to compute its atomic weight, we employ Equation 3.5, with n ∟ ⌐ ⌐KXV

$$A = \frac{\rho V_C N_A}{n}$$

$$= \frac{(8.95 \text{ g/cm}^3)(3.0)(4.0)(3.5)(\times 10^{-24} \text{ cm}^3/\text{unit cell})(6.022 \times 10^{23} \text{ atoms/mol})}{2 \text{ atoms/unit cell}}$$

$$= 113.2 \text{ g/mol}$$

3.49 Convert the (010) and (101) planes into the four-index Miller–Bravais scheme for hexagonal unit cells.

Solution

For (010), h = 0, k = 1, and l = 0, and, from Equation 3.7, the value of i is equal to

$$i = -(h + k) = -(0 + 1) = -1$$
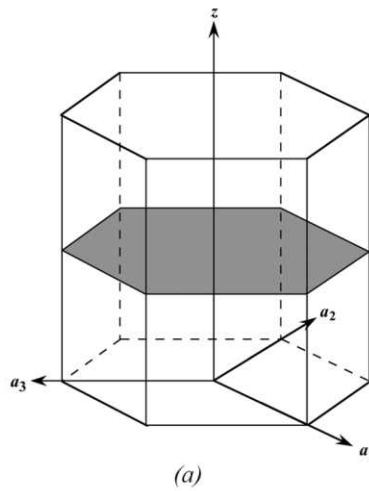
Therefore, the (010) plane becomes $(01\bar{1}0)$.

Now for the (101) plane, h = 1, k = 0, and l = 1, and computation of i using Equation 3.7 leads to

$$i = -(h + k) = -[1 + 0] = -1$$

such that (101) becomes $(10\bar{1}1)$.

3.50 Determine the indices for the planes shown in the hexagonal unit cells below:

Solution

(a)

(a) For this plane, intersections with the a_1, a_2, and z axes are ∞a, ∞a, and c/2 (the plane parallels both a_1 and a_2 axes). In terms of a and c these intersections are ∞, ∞, and ½, the respective reciprocals of which are 0, 0, and 2. This means that
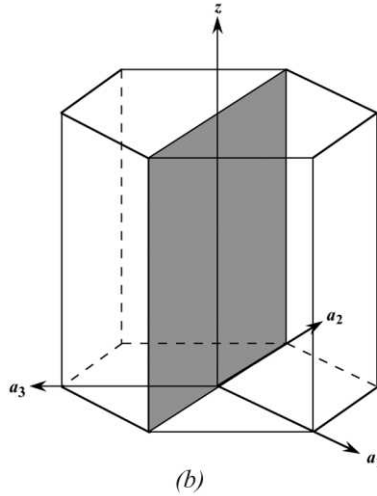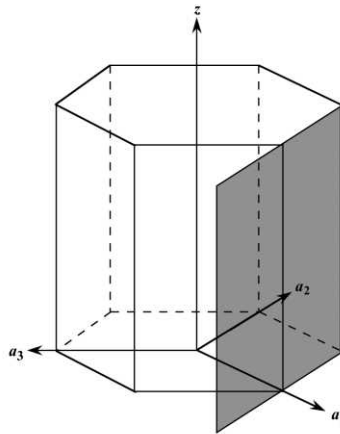
$$h = 0$$
$$k = 0$$
$$l = 2$$

Now, from Equation 3.7, the value of i is

$$i = -(h + k) = -[0 + 0] = 0$$

Hence, this is a (0002) plane.

(b)

(b) This plane passes through the origin of the coordinate axis system; therefore, we translate this plane one unit distance along the x axis, per the sketch shown below:

At this point the plane intersects the a_1, a_2, and z axes at a, ∞a, and ∞c, respectively (the plane parallels both a_2 and z axes). In terms of a and c these intersections are 1, ∞, and ∞, the respective reciprocals of which are 1, 0, and 0. This means that
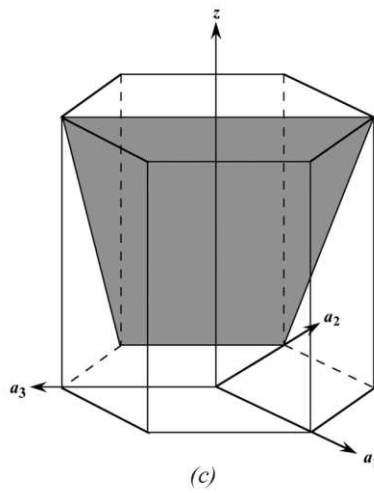
$$h = 1$$
$$k = 0$$
$$l = 0$$

Now, from Equation 3.7, the value of i is

$$i = -(h + k) = -(1 + \ 0) = -1$$

Hence, this is a $(10\bar{1}0)$ plane.

(c)

(c) For this plane, intersections with the a_1, a_2, and z axes are $-a$, a, and c. In terms of a and c these intersections are -1, 1, and 1, the respective reciprocals of which are 0, 1, and 1. This means that
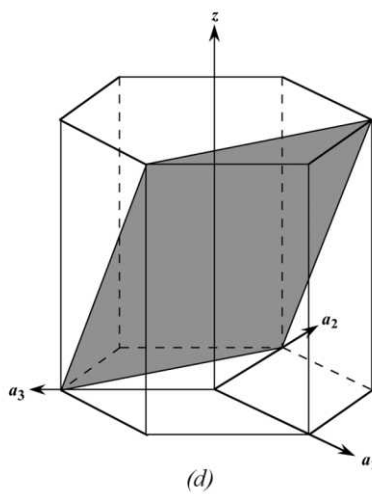
$$h = -1$$
$$k = 1$$
$$l = 1$$

Now, from Equation 3.7, the value of i is

$$i = -(h + k) = -(-1 + 1) = 0$$

Hence, this is a $(\bar{1}101)$ plane.

(d)

(d) For this plane, intersections with the a_1, a_2, and z axes are $-a/2$, a, and c/2, respectively. In terms of a and c these intersections are $-1/2$, 1, and 1/2, the respective reciprocals of which are -2, 1, and 2. This means that

$$h = -2$$
$$k = 1$$
$$l = 2$$

Now, from Equation 3.7, the value of i is

$$i = -(h + k) = -(-2 + 1) = 1$$

Therefore, this is a $(\bar{2}112)$ plane.

3.51 Sketch the $(1\bar{1}01)$ and $(11\bar{2}0)$ planes in a hexagonal unit cell.

Solution

For $(1\bar{1}01)$ the reciprocals of h, k, i, and l are, respectively, $1, -1, \infty$, and 1; thus, this plane is parallel to the a_3 axis, and intersects the a_1 axis at a, the a_2 axis at $-a$, and the z-axis at c. The plane having these intersections is shown in the figure below

$(1\bar{1}01)$
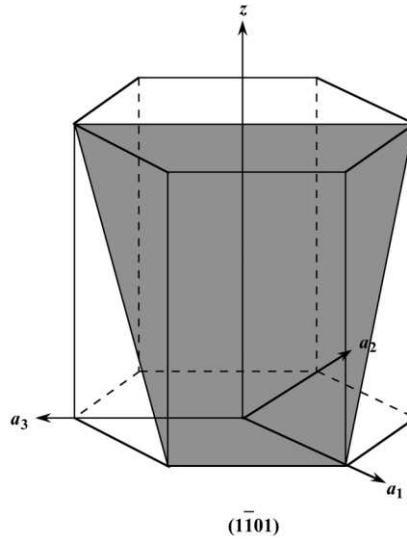
For $(11\bar{2}0)$ the reciprocals of h, k, i, and l are, respectively, $1, 1, -1/2$, and ∞; thus, this plane is parallel to the z axis, and intersects the a_1 axis at a, the a_2 axis at a, and the a_3 axis at $-a/2$. The plane having these intersections is shown in the figure below.
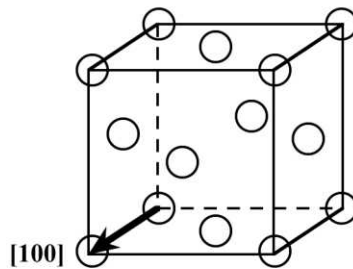

$(11\bar{2}0)$
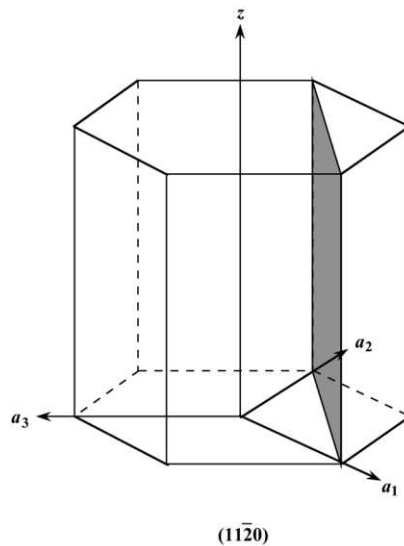
Linear and Planar Densities

3.52   (a) Derive linear density expressions for FCC [100] and [111] directions in terms of the atomic radius R.

(b) Compute and compare linear density values for these same two directions for silver.

Solution

(a) In the figure below is shown a [100] direction within an FCC unit cell.

[100]

For this [100] direction there is one atom at each of the two unit cell corners, and, thus, there is the equivalent of 1 atom that is centered on the direction vector. The length of this direction vector is just the unit cell edge length, $2R\sqrt{2}$ (Equation 3.1). Therefore, the expression for the linear density of this plane is

$$LD_{100} = \frac{\text{number of atoms centered on [100] direction vector}}{\text{length of [100] direction vector}}$$

$$= \frac{1 \text{ atom}}{2\,R\sqrt{2}} = \frac{1}{2\,R\sqrt{2}}$$

An FCC unit cell within which is drawn a [111] direction is shown below.
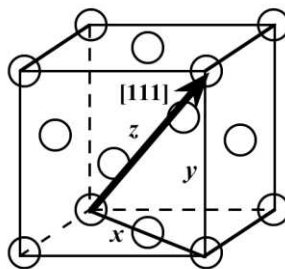
For this [111] direction, the vector shown passes through only the centers of the single atom at each of its ends, and, thus, there is the equivalence of 1 atom that is centered on the direction vector. The length of this direction vector is denoted by z in this figure, which is equal to

$$z = \sqrt{x^2 + y^2}$$

where x is the length of the bottom face diagonal, which is equal to 4R. Furthermore, y is the unit cell edge length, which is equal to $2R\sqrt{2}$ (Equation 3.1). Thus, using the above equation, the length z may be calculated as follows:

$$z = \sqrt{(4R)^2 + (2R\sqrt{2})^2} = \sqrt{24\,R^2} = 2R\sqrt{6}$$

Therefore, the expression for the linear density of this direction is

$$LD_{111} = \frac{\text{number of atoms centered on [111] direction vector}}{\text{length of [111] direction vector}}$$

$$= \frac{1\ \text{atom}}{2R\sqrt{6}} = \frac{1}{2R\sqrt{6}}$$

(b)   From the table inside the front cover, the atomic radius for silver is 0.144 nm. Therefore, the linear density for the [100] direction is

$$LD_{100}(Ag) = \frac{1}{2R\sqrt{2}} = \frac{1}{(2)(0.144\ nm)\sqrt{2}} = 2.46\ nm^{-1} = 2.46 \times 10^9\ m^{-1}$$

While for the [111] direction

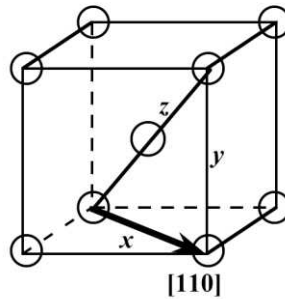$$LD_{111}(Ag) = \frac{1}{2R\sqrt{6}} = \frac{1}{(2)(0.144\ nm)\sqrt{6}} = 1.42\ nm^{-1} = 1.42 \times 10^9\ m^{-1}$$

3.53 (a) Derive linear density expressions for BCC [110] and [111] directions in terms of the atomic radius R.

(b) Compute and compare linear density values for these same two directions for tungsten.

<u>Solution</u>

(a) In the figure below is shown a [110] direction within a BCC unit cell.

[110]

For this [110] direction there is one atom at each of the two unit cell corners, and, thus, there is the equivalence of 1 atom that is centered on the direction vector. The length of this direction vector is denoted by x in this figure, which is equal to

$$x = \sqrt{z^2 - y^2}$$

where y is the unit cell edge length, which, from Equation 3.3 is equal to $\dfrac{4R}{\sqrt{3}}$. Furthermore, z is the length of the unit cell diagonal, which is equal to 4R Thus, using the above equation, the length x may be calculated as follows:

$$x = \sqrt{(4R)^2 - \left(\frac{4R}{\sqrt{3}}\right)^2} = \sqrt{\frac{32R^2}{3}} = 4R\sqrt{\frac{2}{3}}$$

Therefore, the expression for the linear density of this direction is

$$LD_{110} = \frac{\text{number of atoms centered on [110] direction vector}}{\text{length of [110] direction vector}}$$

$$= \frac{1 \text{ atom}}{4R\sqrt{\dfrac{2}{3}}} = \frac{\sqrt{3}}{4R\sqrt{2}}$$

A BCC unit cell within which is drawn a [111] direction is shown below.
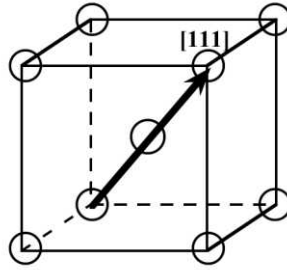
For although the [111] direction vector shown passes through the centers of three atoms, there is an equivalence of only two atoms associated with this unit cell—one-half of each of the two atoms at the end of the vector, in addition to the center atom belongs entirely to the unit cell. Furthermore, the length of the vector shown is equal to 4R, since all of the atoms whose centers the vector passes through touch one another. Therefore, the linear density is equal to

$$LD_{111} = \frac{\text{number of atoms centered on [111] direction vector}}{\text{length of [111] direction vector}}$$

$$= \frac{2 \text{ atoms}}{4R} = \frac{1}{2R}$$

(b) From the table inside the front cover, the atomic radius for tungsten is 0.137 nm. Therefore, the linear density for the [110] direction is

$$LD_{110}(W) = \frac{\sqrt{3}}{4\,R\sqrt{2}} = \frac{\sqrt{3}}{(4)(0.137 \text{ nm})\sqrt{2}} = 2.23 \text{ nm}^{-1} = 2.23 \times 10^9 \text{ m}^{-1}$$
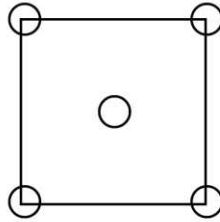
While for the [111] direction

$$LD_{111}(W) = \frac{1}{2\,R} = \frac{1}{(2)(0.137 \text{ nm})} = 3.65 \text{ nm}^{-1} = 3.65 \times 10^9 \text{ m}^{-1}$$

3.54 (a) Derive planar density expressions for FCC (100) and (111) planes in terms of the atomic radius R.

(b) Compute and compare planar density values for these same two planes for nickel.

Solution

(a) In the figure below is shown a (100) plane for an FCC unit cell.

For this (100) plane there is one atom at each of the four cube corners, each of which is shared with four adjacent unit cells, while the center atom lies entirely within the unit cell. Thus, there is the equivalence of 2 atoms associated with this FCC (100) plane. The planar section represented in the above figure is a square, wherein the side lengths are equal to the unit cell edge length, $2R\sqrt{2}$ [Equation (3.1)]; and, thus, the area of this square is just $(2R\sqrt{2})^2 = 8R^2$. Hence, the planar density for this (100) plane is just

$$PD_{100} = \frac{\text{number of atoms centered on (100) plane}}{\text{area of (100) plane}}$$

$$= \frac{2 \text{ atoms}}{8R^2} = \frac{1}{4R^2}$$

That portion of an FCC (111) plane contained within a unit cell is shown below.
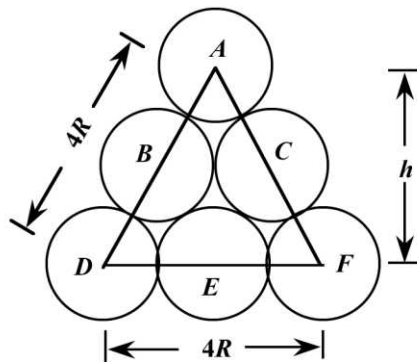
There are six atoms whose centers lie on this plane, which are labeled A through F. One-sixth of each of atoms A, D, and F are associated with this plane (yielding an equivalence of one-half atom), with one-half of each of atoms B, C, and E (or an equivalence of one and one-half atoms) for a total equivalence of two atoms. Now, the area of the triangle shown in the above figure is equal to one-half of the product of the base length and the height, h. If we consider half of the triangle, then

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

which leads to $h = 2R\sqrt{3}$. Thus, the area is equal to

$$Area = \frac{4R(h)}{2} = \frac{(4R)(2R\sqrt{3})}{2} = 4R^2\sqrt{3}$$

And, thus, the planar density is

$$PD_{111} = \frac{\text{number of atoms centered on (111) plane}}{\text{area of (111) plane}}$$

$$= \frac{2 \text{ atoms}}{4R^2\sqrt{3}} = \frac{1}{2R^2\sqrt{3}}$$

(b) From the table inside the front cover, the atomic radius for nickel is 0.125 nm. Therefore, the planar density for the (100) plane is

$$PD_{100}(Ni) = \frac{1}{4R^2} = \frac{1}{4(0.125 \text{ nm})^2} = 16.00 \text{ nm}^{-2} = 1.600 \times 10^{19} \text{ m}^{-2}$$

While for the (111) plane

$$PD_{111}(Ni) = \frac{1}{2R^2\sqrt{3}} = \frac{1}{2\sqrt{3}(0.125 \text{ nm})^2} = 18.48 \text{ nm}^{-2} = 1.848 \times 10^{19} \text{ m}^{-2}$$

3.55 (a) Derive planar density expressions for BCC (100) and (110) planes in terms of the atomic radius R.
(b) Compute and compare planar density values for these same two planes for vanadium.

Solution

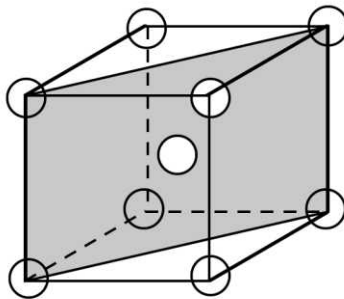(a) A BCC unit cell within which is drawn a (100) plane is shown below.
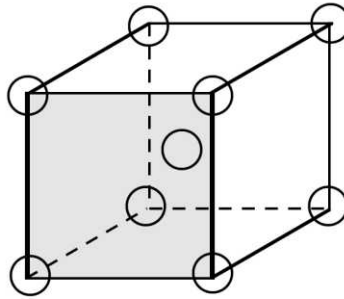
For this (100) plane there is one atom at each of the four cube corners, each of which is shared with four adjacent unit cells. Thus, there is the equivalence of 1 atom associated with this BCC (100) plane. The planar section represented in the above figure is a square, wherein the side lengths are equal to the unit cell edge length, $\dfrac{4R}{\sqrt{3}}$ (Equation 3.4); and, thus, the area of this square is just $\left(\dfrac{4R}{\sqrt{3}}\right)^2 = \dfrac{16\,R^2}{3}$. Hence, the planar density for this (100) plane is just

$$PD_{100} = \frac{\text{number of atoms centered on (100) plane}}{\text{area of (100) plane}}$$

$$= \frac{1\ \text{atom}}{\dfrac{16\ R^2}{3}} = \frac{3}{16\ R^2}$$

A BCC unit cell within which is drawn a (110) plane is shown below.

For this (110) plane there is one atom at each of the four cube corners through which it passes, each of which is shared with four adjacent unit cells, while the center atom lies entirely within the unit cell. Thus, there is the equivalence of 2 atoms associated with this BCC (110) plane. The planar section represented in the above figure is a rectangle, as noted in the figure below.
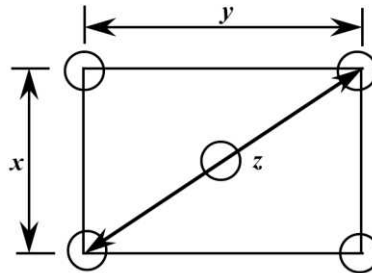
From this figure, the area of the rectangle is the product of x and y. The length x is just the unit cell edge length, which for BCC (Equation 3.3) is $\dfrac{4R}{\sqrt{3}}$. Now, the diagonal length z is equal to 4R. For the triangle bounded by the lengths x, y, and z

$$y = \sqrt{z^2 - x^2}$$

Or

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

Thus, in terms of R, the area of this (110) plane is just

$$\text{Area}(110) = xy = \left(\frac{4R}{\sqrt{3}}\right)\left(\frac{4R\sqrt{2}}{\sqrt{3}}\right) = \frac{16R^2\sqrt{2}}{3}$$

And, finally, the planar density for this (110) plane is just

$$PD_{110} = \frac{\text{number of atoms centered on (110) plane}}{\text{area of (110) plane}}$$

$$= \frac{2 \text{ atoms}}{\dfrac{16R^2\sqrt{2}}{3}} = \frac{3}{8R^2\sqrt{2}}$$

(b) From the table inside the front cover, the atomic radius for vanadium is 0.132 nm. Therefore, the planar density for the (100) plane is

$$PD_{100}(V) = \frac{3}{16\,R^2} = \frac{3}{16\,(0.132\ nm)^2} = 10.76\ nm^{-2} = 1.076 \times 10^{19}\ m^{-2}$$
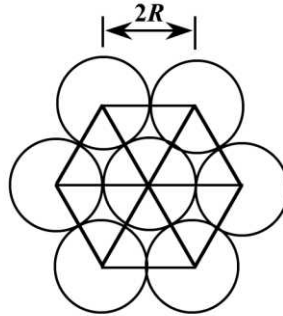
While for the (110) plane

$$PD_{110}(V) = \frac{3}{8\,R^2\sqrt{2}} = \frac{3}{8\,(0.132\ nm)^2\sqrt{2}} = 15.22\ nm^{-2} = 1.522 \times 10^{19}\ m^{-2}$$

3.56 (a) Derive the planar density expression for the HCP (0001) plane in terms of the atomic radius R.

(b) Compute the planar density value for this same plane for magnesium.

<u>Solution</u>

(a) A (0001) plane for an HCP unit cell is show below.

Each of the 6 perimeter atoms in this plane is shared with three other unit cells, whereas the center atom is shared with no other unit cells; this gives rise to three equivalent atoms belonging to this plane.

In terms of the atomic radius R, the area of each of the 6 equilateral triangles that have been drawn is $R^2\sqrt{3}$, or the total area of the plane shown is $6R^2\sqrt{3}$. And the planar density for this (0001) plane is equal to

$$PD_{0001} = \frac{\text{number of atoms centered on (0001) plane}}{\text{area of (0001) plane}}$$

$$= \frac{3 \text{ atoms}}{6R^2\sqrt{3}} = \frac{1}{2R^2\sqrt{3}}$$

(b) From the table inside the front cover, the atomic radius for magnesium is 0.160 nm. Therefore, the planar density for the (0001) plane is

$$PD_{0001}(Mg) = \frac{1}{2R^2\sqrt{3}} = \frac{1}{2(0.160 \text{ nm})^2\sqrt{3}} = 11.28 \text{ nm}^{-2} = 1.128 \times 10^{19} \text{ m}^{-2}$$

Polycrystalline Materials

3.57 Explain why the properties of polycrystalline materials are most often isotropic.

<u>Solution</u>

Although each individual grain in a polycrystalline material may be anisotropic, if the grains have random orientations, then the solid aggregate of the many anisotropic grains will behave isotropically.

X-ray Diffraction: Determination of Crystal Structures

3.58 Using the data for molybdenum in Table 3.1, compute the interplanar spacing for the (111) set of planes.

<u>Solution</u>

From the Table 3.1, molybdenum has a BCC crystal structure and an atomic radius of 0.1363 nm. Using Equation (3.3), the lattice parameter a may be computed as

$$a = \frac{4R}{\sqrt{3}} = \frac{(4)(0.1363 \ \text{nm})}{\sqrt{3}} = 0.3148 \ \text{nm}$$

Now, the interplanar spacing d_{111} maybe determined using Equation 3.14 as

$$d_{111} = \frac{a}{\sqrt{(1)^2 + (1)^2 + (1)^2}} = \frac{0.3148 \ \text{nm}}{\sqrt{3}} = 0.1817 \ \text{nm}$$

3.59 Determine the expected diffraction angle for the first-order reflection from the (113) set of planes for FCC platinum when monochromatic radiation of wavelength 0.1542 nm is used.

Solution

We first calculate the lattice parameter using Equation 3.1 and the value of R (0.1387 nm) cited in Table 3.1, as follows:

$$a = 2R\sqrt{2} = (2)(0.1387 \text{ nm})(\sqrt{2}) = 0.3923 \text{ nm}$$

Next, the interplanar spacing for the (113) set of planes may be determined using Equation 3.14 according to

$$d_{113} = \frac{a}{\sqrt{(1)^2 + (1)^2 + (3)^2}} = \frac{0.3923 \text{ nm}}{\sqrt{11}} = 0.1183 \text{ nm}$$

And finally, employment of Equation 3.13 yields the diffraction angle as

$$\sin \theta = \frac{n\lambda}{2d_{113}} = \frac{(1)(0.1542 \text{ nm})}{(2)(0.1183 \text{ nm})} = 0.652$$

Which leads to

$$\theta = \sin^{-1}(0.652) = 40.69°$$

And, finally

$$2\theta = (2)(40.69°) = 81.38°$$

3.60 Using the data for aluminum in Table 3.1, compute the interplanar spacings for the (110) and (221) sets of planes.

<u>Solution</u>

From the table, aluminum has an FCC crystal structure and an atomic radius of 0.1431 nm. Using Equation 3.1 the lattice parameter, a, may be computed as

$$a = 2R\sqrt{2} = (2)(0.1431 \text{ nm})(\sqrt{2}) = 0.4047 \text{ nm}$$

Now, the d_{110} interplanar spacing may be determined using Equation 3.14 as

$$d_{110} = \frac{a}{\sqrt{(1)^2 + (1)^2 + (0)^2}} = \frac{0.4047 \text{ nm}}{\sqrt{2}} = 0.2862 \text{ nm}$$

And, similarly for d_{221}

$$d_{221} = \frac{a}{\sqrt{(2)^2 + (2)^2 + (1)^2}} = \frac{0.4047 \text{ nm}}{\sqrt{9}} = 0.1349 \text{ nm}$$

3.61 The metal iridium has an FCC crystal structure. If the angle of diffraction for the (220) set of planes occurs at 69.22° (first-order reflection) when monochromatic x-radiation having a wavelength of 0.1542 nm is used, compute (a) the interplanar spacing for this set of planes, and (b) the atomic radius for an iridium atom.

Solution

(a) From the data given in the problem, and realizing that 69.22° = 2θ, the interplanar spacing for the (220) set of planes for iridium may be computed using Equation 3.13 as

$$d_{220} = \frac{n\lambda}{2 \sin \theta} = \frac{(1)(0.1542 \text{ nm})}{(2)\left(\sin \dfrac{69.22 \text{ °}}{2} \right)} = 0.1357 \text{ nm}$$

(b) In order to compute the atomic radius we must first determine the lattice parameter, a, using Equation 3.14, and then R from Equation 3.1 since Ir has an FCC crystal structure. Therefore,

$$a = d_{220}\sqrt{(2)^2 + (2)^2 + (0)^2} = (0.1357 \text{ nm})(\sqrt{8}) = 0.3838 \text{ nm}$$

And, from Equation 3.1

$$R = \frac{a}{2\sqrt{2}} = \frac{0.3838 \text{ nm}}{2\sqrt{2}} = 0.1357 \text{ nm}$$

3.62 The metal rubidium has a BCC crystal structure. If the angle of diffraction for the (321) set of planes occurs at 27.00° (first-order reflection) when monochromatic x-radiation having a wavelength of 0.0711 nm is used, compute (a) the interplanar spacing for this set of planes, and (b) the atomic radius for the rubidium atom.

<u>Solution</u>

(a) From the data given in the problem, and realizing that 27.00° = 2θ, the interplanar spacing for the (321) set of planes for Rb may be computed using Equation 3.13 as follows:

$$d_{321} = \frac{n\lambda}{2\sin\theta} = \frac{(1)(0.0711 \text{ nm})}{(2)\left(\sin\dfrac{27.00°}{2}\right)} = 0.1523 \text{ nm}$$

(b) In order to compute the atomic radius we must first determine the lattice parameter, a, using Equation 3.14, and then R from Equation 3.3 since Rb has a BCC crystal structure. Therefore,

$$a = d_{321}\sqrt{(3)^2 + (2)^2 + (1)^2} = (0.1523 \text{ nm})\left(\sqrt{14}\right) = 0.5700 \text{ nm}$$

And, from Equation 3.3

$$R = \frac{a\sqrt{3}}{4} = \frac{(0.5700 \text{ nm})\sqrt{3}}{4} = 0.2468 \text{ nm}$$

3.63 For which set of crystallographic planes will a first-order diffraction peak occur at a diffraction angle of 46.21° for BCC iron when monochromatic radiation having a wavelength of 0.0711 nm is used?

<u>Solution</u>

The first step to solve this problem is to compute the interplanar spacing using Equation 3.13. Thus,

$$d_{hkl} = \frac{n\lambda}{2 \sin \theta} = \frac{(1)(0.0711 \ nm)}{(2)\left(\sin \dfrac{46.21°}{2} \right)} = 0.0906 \ nm$$

Now, employment of both Equations 3.14 and 3.3 (since Fe's crystal structure is BCC), and the value of R for iron from Table 3.1 (0.1241 nm) leads to

$$\sqrt{h^2 + k^2 + l^2} = \frac{a}{d_{hkl}} = \frac{4R}{d_{hkl}\sqrt{3}}$$

$$= \frac{(4)(0.1241 \ nm)}{(0.0906 \ nm)(\sqrt{3})} = 3.163$$

This means that

$$h^2 + k^2 + l^2 = (3.163)^2 = 10.0$$

By trial and error, the only three integers having a sum that is even, and the sum of the squares of which equals 10.0 are 3, 1, and 0. Therefore, the set of planes responsible for this diffraction peak are the (310) ones.

3.64   Figure 3.22 shows an x-ray diffraction pattern for α-iron taken using a diffractometer and monochromatic x-radiation having a wavelength of 0.1542 nm; each diffraction peak on the pattern has been indexed. Compute the interplanar spacing for each set of planes indexed; also determine the lattice parameter of Fe for each of the peaks.
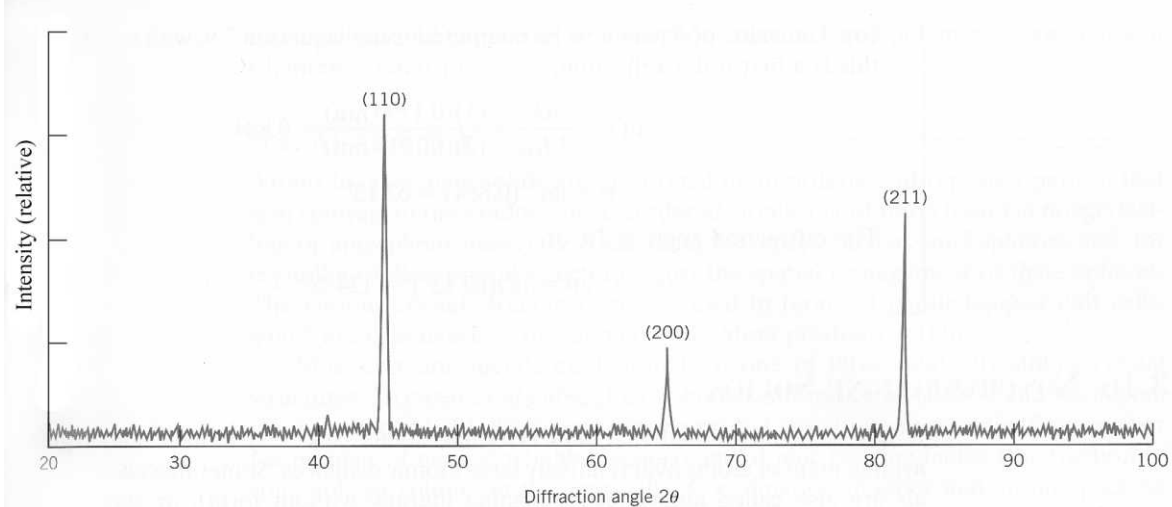

FIGURE 3.22 Diffraction pattern for polycrystalline α-iron.

Solution

For each peak, in order to compute the interplanar spacing and the lattice parameter we must employ Equations 3.14 and 3.13, respectively. The first peak of Figure 3.22, which results from diffraction by the (110) set of planes, occurs at 2θ = 45.0°; the corresponding interplanar spacing for this set of planes, using Equation 3.13, is equal to

$$d_{110} = \frac{n\lambda}{2 \sin \theta} = \frac{(1)(0.1542 \text{ nm})}{(2)\left(\sin \dfrac{45.0°}{2} \right)} = 0.2015 \text{ nm}$$

And, from Equation 3.14, the lattice parameter a is determined as

$$a = d_{hkl}\sqrt{(h)^2 + (k)^2 + (l)^2} = d_{110}\sqrt{(1)^2 + (1)^2 + (0)^2}$$

$$= (0.2015 \text{ nm})\sqrt{2} = 0.2850 \text{ nm}$$

Similar computations are made for the other peaks which results are tabulated below:

Peak Index	2θ	d_{hkl}(nm)	a (nm)
200	65.1	0.1433	0.2866
211	82.8	0.1166	0.2856

3.65   The diffraction peaks shown in Figure 3.22 are indexed according to the reflection rules for BCC (i.e., the sum $h + k + l$ must be even). Cite the $h, k,$ and l indices for the first four diffraction peaks for FCC crystals consistent with $h, k,$ and l all being either odd or even.

<u>Solution</u>

The first four diffraction peaks that will occur for FCC consistent with $h, k,$ and l all being odd or even are (111), (200), (220), and (311).

3.66 Figure 3.25 shows the first four peaks of the x-ray diffraction pattern for copper, which has an FCC crystal structure; monochromatic x-radiation having a wavelength of 0.1542 nm was used.

(a) Index (i.e., give h, k, and l indices) for each of these peaks.

(b) Determine the interplanar spacing for each of the peaks.

(c) For each peak, determine the atomic radius for Cu and compare these with the value presented in Table 3.1.
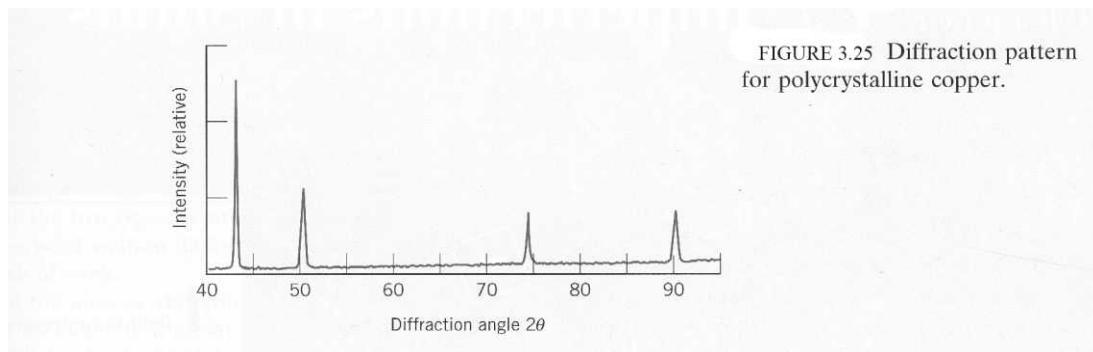

FIGURE 3.25 Diffraction pattern for polycrystalline copper.

Solution

(a) Since Cu has an FCC crystal structure, only those peaks for which h, k, and l are all either odd or even will appear. Therefore, the first peak results by diffraction from (111) planes.

(b) For each peak, in order to calculate the interplanar spacing we must employ Equation 3.13. For the first peak which occurs at 43.8°

$$d_{111} = \frac{n\lambda}{2 \sin \theta} = \frac{(1)(0.1542 \text{ nm})}{(2)\left(\sin \dfrac{43.8°}{2}\right)} = 0.2067 \text{ nm}$$

(c) Employment of Equations 3.14 and 3.1 is necessary for the computation of R for Cu as

$$R = \frac{a}{2\sqrt{2}} = \frac{(d_{hkl})\sqrt{(h)^2 + (k)^2 + (l)^2}}{2\sqrt{2}}$$

$$= \frac{(0.2067 \text{ nm})\sqrt{(1)^2 + (1)^2 + (1)^2}}{2\sqrt{2}}$$

$$= 0.1266 \text{ nm}$$

Similar computations are made for the other peaks which results are tabulated below:

Peak Index	2θ	d_{hkl}(nm)	R (nm)
200	50.8	0.1797	0.1271
220	74.4	0.1275	0.1275
311	90.4	0.1087	0.1274

Noncrystalline Solids

3.67 Would you expect a material in which the atomic bonding is predominantly ionic in nature to be more or less likely to form a noncrystalline solid upon solidification than a covalent material? Why? (See Section 2.6.)

<u>Solution</u>

A material in which atomic bonding is predominantly ionic in nature is less likely to form a noncrystalline solid upon solidification than a covalent material because covalent bonds are directional whereas ionic bonds are nondirectional; it is more difficult for the atoms in a covalent material to assume positions giving rise to an ordered structure.