CHAPTER 3

THE STRUCTURE OF CRYSTALLINE SOLIDS

PROBLEM SOLUTIONS

Fundamental Concepts

3.1 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.

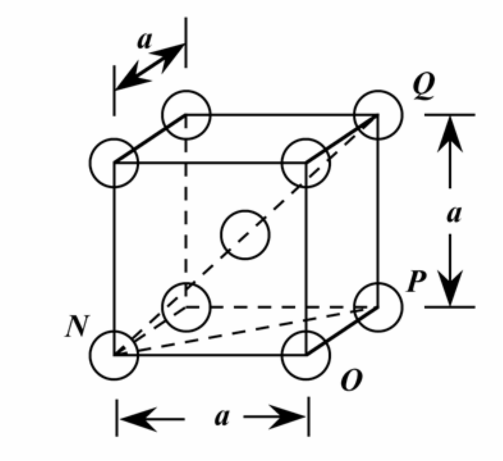
Unit Cells

Metallic Crystal Structures

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

$$V_C = 16R^3\sqrt{2} = (16)\left(0.175 \times 10^{-9}\ \text{m}\right)^3\left(\sqrt{2}\right) = 1.213 \times 10^{-28}\ \text{m}^3$$

3.3 This problem calls for a demonstration of the relationship $a = \frac{4R}{\sqrt{3}}$ for BCC. 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*,

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

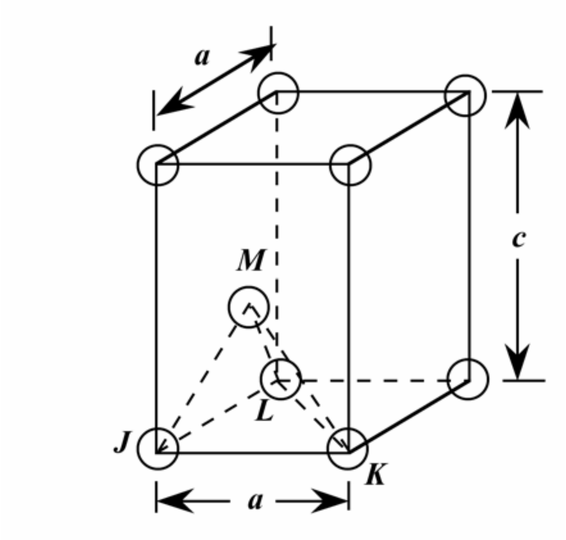
But $\overline{NQ} = 4R$, *R* being the atomic radius. Also, $\overline{QP} = a$. Therefore,

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

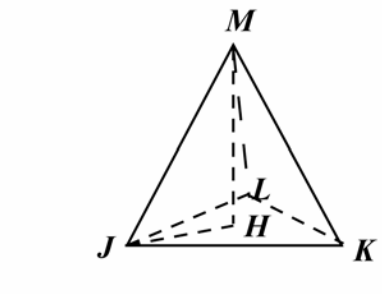
or

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

3.4 We are asked to show that the ideal *c/a* ratio for HCP 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,

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

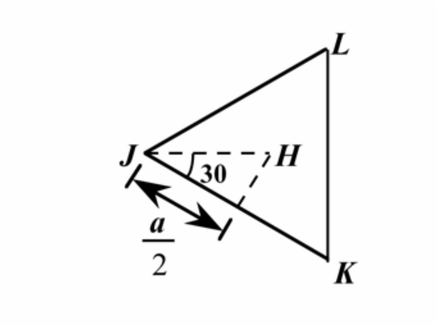
where *R* is the atomic radius. Furthermore, from triangle *JHM*,

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

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 We are asked to show that the atomic packing factor for BCC is 0.68. The atomic packing factor is defined as the ratio of sphere volume to the total unit cell volume, or

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

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

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

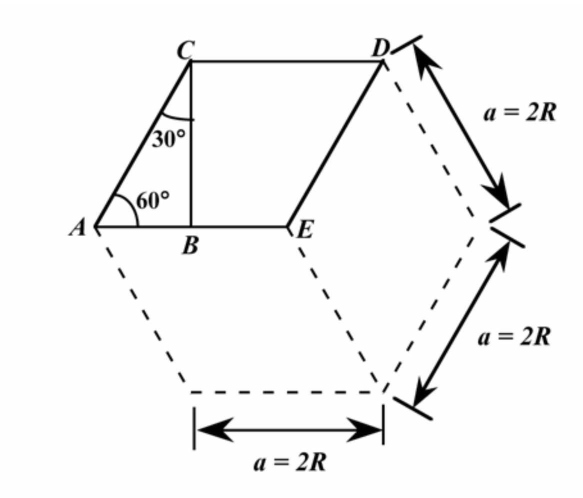
Thus,

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

3.6 This problem calls for a demonstration that the APF for HCP is 0.74. Again, 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 2*R*, and

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

Thus, the base area is just

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

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

$$V_C = (\text{AREA})(c) = 6R^2c\sqrt{3} = \left(6R^2\sqrt{3}\right)(2)(1.633)R = 12\sqrt{3}\,(1.633)\,R^3$$

Thus,

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

Density Computations

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

$$\rho = \frac{nA_{\mathrm{Mo}}}{V_C N_{\mathrm{A}}}$$

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

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

Thus,

$$\rho = \frac{nA_{\mathrm{Mo}}}{\left(\frac{4R}{\sqrt{3}}\right)^3 N_{\mathrm{A}}}$$

$$= \frac{(2 \text{ atoms/unit cell})(95.94 \text{ g/mol})}{\left[(4)\left(0.1363 \times 10^{-7} \text{ cm}\right)^3/\sqrt{3}\right]^3 /(\text{unit cell})\left(6.023 \times 10^{23} \text{ atoms/mol}\right)}$$

$$= 10.21 \text{ g/cm}^3$$

The value given inside the front cover is 10.22 g/cm^3.

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

$$\rho = \frac{nA_{\text{Pd}}}{V_C N_{\text{A}}}$$

$$= \frac{nA_{\text{Pd}}}{(16R^3\sqrt{2})N_{\text{A}}}$$

And solving for R from the above expression yields

$$R = \left(\frac{nA_{\text{Pd}}}{16\rho N_{\text{A}}\sqrt{2}}\right)^{1/3}$$

$$= \left[\frac{(4\text{ atoms/unit cell})(106.4\text{ g/mol})}{(16)(12.0\text{ g/cm}^3)(6.023 \times 10^{23}\text{ atoms/mol})(\sqrt{2})}\right]^{1/3}$$

$$= 1.38 \times 10^{-8}\text{ cm} = 0.138\text{ nm}$$

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

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

Since, from Equation 3.5

$$\rho = \frac{nA_{\text{Ta}}}{V_C N_{\text{A}}}$$

$$= \frac{nA_{\text{Ta}}}{\left(\frac{64R^3}{3\sqrt{3}}\right) N_{\text{A}}}$$

and solving for R the previous equation

$$R = \left(\frac{3\sqrt{3}nA_{\text{Ta}}}{64\rho N_{\text{A}}}\right)^{1/3}$$

$$= \left[\frac{(3\sqrt{3})(2 \text{ atoms/unit cell})(180.9 \text{ g/mol})}{(64)(16.6 \text{ g/cm}^3)(6.023 \times 10^{23} \text{ atoms/mol})}\right]^{1/3}$$

$$= 1.43 \times 10^{-8} \text{ cm} = 0.143 \text{ nm}$$

3.10 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 3.23). Therefore, employment of Equation 3.5 yields

$$\rho = \frac{nA}{V_C N_\mathrm{A}} = \frac{nA}{(2R)^3 N_\mathrm{A}}$$

$$= \frac{(1 \text{ atom/unit cell})(74.5 \text{ g/mol})}{\left\{\left[(2)\left(1.45 \times 10^{-8} \text{ cm}\right)\right]^3 /(\text{unit cell})\right\}\left(6.023 \times 10^{23} \text{ atoms/mol}\right)}$$

$$5.07 \text{ g/cm}^3$$

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

$$V_C = \frac{nA_{\text{Ti}}}{\rho N_{\text{A}}}$$

Now, for HCP, n = 6 atoms/unit cell, and for Ti, A_{Ti} = 47.9 g/mol. Thus,

$$V_C = \frac{(6 \text{ atoms/unit cell})(47.9 \text{ g/mol})}{\left(4.51 \text{ g/cm}^3\right)\left(6.023 \text{ x } 10^{23} \text{ atoms/mol}\right)}$$

$$= 1.058 \text{ x } 10^{-22} \text{ cm}^3\text{/unit cell} = 1.058 \text{ x } 10^{-28} \text{ m}^3\text{/unit cell}$$

(b) From part of the solution to Problem 3.6, for HCP

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

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

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

but, since $c = 1.58a$

$$V_C = \frac{3\sqrt{3}\,(1.58)\,a^3}{2} = 1.058 \text{ x } 10^{-22} \text{ cm}^3\text{/unit cell}$$

Now, solving for a

$$a = \left[\frac{(2)\left(1.058 \text{ x } 10^{-22} \text{ cm}^3\right)}{(3)\left(\sqrt{3}\right)(1.58)}\right]^{1/3}$$

$$= 2.96 \text{ x } 10^{-8} \text{ cm} = 0.296 \text{ nm}$$

And finally

$$c = 1.58a = (1.58)(0.296 \text{ nm}) = 0.468 \text{ nm}$$

3.12 This problem asks that we calculate the theoretical densities of Al, Ni, Mg, and W.

Since Al has an FCC crystal structure, $n = 4$, and $V_C = 16R^3\sqrt{2}$ (Equation 3.4). Also, $R = 0.143$ nm (1.43×10^{-8} cm) and $A_{\mathrm{Al}} = 26.98$ g/mol. Employment of Equation 3.5 yields

$$\rho = \frac{nA_{\mathrm{Al}}}{V_C N_{\mathrm{A}}}$$

$$= \frac{(4\ \text{atoms/unit cell})(26.98\ \text{g/mol})}{\left\{\left[(2)(1.43 \times 10^{-8}\ \text{cm})(\sqrt{2})\right]^3/(\text{unit cell})\right\}(6.023 \times 10^{23}\ \text{atoms/mol})}$$

$$= 2.71\ \text{g/cm}^3$$

The value given in the table inside the front cover is 2.71 g/cm^3.

Nickel also has an FCC crystal structure and therefore

$$\rho = \frac{(4\ \text{atoms/unit cell})(58.69\ \text{g/mol})}{\left\{\left[(2)(1.25 \times 10^{-8}\ \text{cm})(\sqrt{2})\right]^3/(\text{unit cell})\right\}(6.023 \times 10^{23}\ \text{atoms/mol})}$$

$$= 8.82\ \text{g/cm}^3$$

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

Magnesium has an HCP crystal structure, and from the solution to Problem 3.6,

$$V_C = \frac{3\sqrt{3}\,a^2c}{2}$$

and, since $c = 1.624a$ and $a = 2R = 2(1.60 \times 10^{-8}\ \text{cm}) = 3.20 \times 10^{-8}$ cm

$$V_C = \frac{(3\sqrt{3})(1.624)(3.20 \times 10^{-8}\ \text{cm})^3}{2} = 1.38 \times 10^{-22}\ \text{cm}^3/\text{unit cell}$$

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

$$\rho = \frac{nA_{\mathrm{Mg}}}{V_C N_{\mathrm{A}}}$$

$$= \frac{(6 \text{ atoms/unit cell})(24.31 \text{ g/mol})}{\left(1.38 \times 10^{-22} \text{ cm}^3\text{/unit cell}\right)\left(6.023 \times 10^{23} \text{ atoms/mol}\right)}$$

$$= 1.75 \text{ g/cm}^3$$

The value given in the table is 1.74 g/cm^3.

Tungsten has a BCC crystal structure for which $n = 2$ and $a = \frac{4R}{\sqrt{3}}$ (Equation 3.3); also A_W = 183.85 g/mol and R = 0.137 nm. Therefore, employment of Equation 3.5 leads to

$$\rho = \frac{(2 \text{ atoms/unit cell})(183.85 \text{ g/mol})}{\left\{\left[\frac{(4)\left(1.37 \times 10^{-8} \text{ cm}\right)}{\sqrt{3}}\right]^3 \text{/(unit cell)}\right\}\left(6.023 \times 10^{23} \text{ atoms/mol}\right)}$$

$$= 19.3 \text{ g/cm}^3$$

The value given in the table is 19.3 g/cm^3.

3.13 In order to determine whether Nb 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 92.91 g/mol. Thus, for FCC (employing Equation 3.5)

$$\rho = \frac{nA_{\mathrm{Nb}}}{a^3 N_{\mathrm{A}}} = \frac{nA_{\mathrm{Nb}}}{(2R\sqrt{2})^3 N_{\mathrm{A}}}$$

$$= \frac{(4 \text{ atoms/unit cell})(92.91 \text{ g/mol})}{\left\{\left[(2)(1.43 \times 10^{-8}\text{ cm})(\sqrt{2})\right]^3/(\text{unit cell})\right\}(6.023 \times 10^{23}\text{ atoms/mol})}$$

$$= 9.33 \text{ g/cm}^3$$

For BCC, $n = 2$, and $a = \frac{4R}{\sqrt{3}}$ (Equation 3.3), thus

$$\rho = \frac{nA_{\mathrm{Nb}}}{\left(\frac{4R}{\sqrt{3}}\right)^3 N_{\mathrm{A}}}$$

$$\rho = \frac{(2 \text{ atoms/unit cell})(92.91 \text{ g/mol})}{\left\{\left[\frac{(4)(1.43 \times 10^{-8}\text{ cm})}{\sqrt{3}}\right]^3/(\text{unit cell})\right\}(6.023 \times 10^{23}\text{ atoms/mol})}$$

$$= 8.57 \text{ g/cm}^3$$

which is the value provided in the problem statement. Therefore, Nb has a BCC crystal structure.

3.14 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 $\frac{4R}{\sqrt{3}}$.

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

$$\rho = \frac{nA_{\mathrm{A}}}{V_C N_{\mathrm{A}}}$$

$$= \frac{nA_{\mathrm{A}}}{\left(\frac{4R}{\sqrt{3}}\right)^3 N_{\mathrm{A}}}$$

$$= \frac{(2\text{ atoms/unit cell})(43.1\text{ g/mol})}{\left\{\left[\frac{(4)(1.22 \times 10^{-8}\text{ cm})}{\sqrt{3}}\right]^3 /(\text{unit cell})\right\}(6.023 \times 10^{23}\text{ atoms/mol})}$$

$$= 6.40\text{ g/cm}^3$$

Therefore, its crystal structure is BCC.

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

$$\rho = \frac{nA_{\mathrm{B}}}{(2a)^3 N_{\mathrm{A}}}$$

$$= \frac{(1\text{ atom/unit cell})(184.4\text{ g/mol})}{\left\{\left[(2)(1.46 \times 10^{-8}\text{ cm})\right]^3 /(\text{unit cell})\right\}(6.023 \times 10^{23}\text{ atoms/mol})}$$

$$= 12.3\text{ g/cm}^3$$

Therefore, its crystal structure is simple cubic.

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

$$\rho = \frac{nA_{\mathrm{C}}}{\left(\dfrac{4R}{\sqrt{3}}\right)^3 N_{\mathrm{A}}}$$

$$= \frac{(2\text{ atoms/unit cell})(91.6\text{ g/mol})}{\left\{\left[\dfrac{(4)\left(1.37 \times 10^{-8}\text{ cm}\right)}{\sqrt{3}}\right]^3 /(\text{unit cell})\right\}\left(6.023 \times 10^{23}\text{ atoms/mol}\right)}$$

$$= 9.60\text{ g/cm}^3$$

Therefore, its crystal structure is BCC.

3.15 In order to determine the APF for U, we need to compute both the unit cell volume (V_C) which is just the product of the three unit cell parameters, 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

$$n = \frac{\rho V_C N_\mathrm{A}}{A_\mathrm{U}}$$

$$= \frac{(19.05\ \mathrm{g/cm^3})(2.86)(5.87)(4.95)\left(\times\ 10^{-24}\ \mathrm{cm^3}\right)\left(6.023\ \times\ 10^{23}\ \mathrm{atoms/mol}\right)}{238.03\ \mathrm{g/mol}}$$

$$= 4.01\ \text{atoms/unit cell}$$

Therefore

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

$$= \frac{(4)\left[\dfrac{4}{3}(\pi)(1.385\text{Źx } 10^{8}\ \mathrm{cm})^3\right]}{(2.86)(5.87)(4.95)\left(\text{xŹ}10^{24}\ \mathrm{cm^3}\right)}$$

$$= 0.536$$

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

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

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

$$n = \frac{(\text{APF})\, a^2 c}{\frac{4}{3}\pi R^3}$$

$$= \frac{(0.693)(4.59)^2(4.95)\left(10^{-24}\ \text{cm}^3\right)}{\frac{4}{3}\pi\left(1.625 \times 10^{-8}\ \text{cm}\right)^3}$$

$$= 4.0 \text{ atoms/unit cell}$$

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

$$\rho = \frac{nA_{\text{In}}}{a^2 c\, N_{\text{A}}}$$

$$= \frac{(4\ \text{atoms/unit cell})(114.82\ \text{g/mol})}{\left[\left(4.59 \times 10^{-8}\ \text{cm}\right)^2\left(4.95 \times 10^{-8}\ \text{cm}\right)/\text{unit cell}\right]\left(6.023 \times 10^{23}\ \text{atoms/mol}\right)}$$

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

3. 17 (a) We are asked to calculate the unit cell volume for Be. For HCP, from the solution to Problem 3.6

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

But, $c = 1.568a$, and $a = 2R$, or $c = 3.14R$, and

$$V_C = (6)(3.14)\ R^3\sqrt{3}$$

$$= (6)(3.14)(\sqrt{3})\left[0.1143 \times 10^{-7}\ \text{cm}\right]^3 = 4.87 \times 10^{-23}\ \text{cm}^3/\text{unit cell}$$

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

$$\rho = \frac{nA_{\text{Be}}}{V_C N_{\text{A}}}$$

For HCP, $n = 6$ atoms/unit cell, and for Be, $A_{\text{Be}} = 9.01$ g/mol (as noted inside the front cover). Thus,

$$\rho = \frac{(6\ \text{atoms/unit cell})(9.01\ \text{g/mol})}{\left(4.87 \times 10^{-23}\ \text{cm}^3/\text{unit cell}\right)\left(6.023 \times 10^{23}\ \text{atoms/mol}\right)}$$

$$= 1.84\ \text{g/cm}^3$$

The value given in the literature is 1.85 g/cm^3.

3.18 This problem calls for us to compute the atomic radius for Mg. In order to do this we must use Equation 3.5, as well as the expression which relates the atomic radius to the unit cell volume for HCP; from Problem 3.6 it was shown that

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

In this case $c = 1.624a$, but, for HCP, $a = 2R$, which means that

$$V_C = 6R^2(1.624)(2R)\sqrt{3} = (1.624)\left(12\sqrt{3}\right)R^3$$

And from Equation 3.5, the density is equal to

$$\rho = \frac{nA_{\mathrm{Mg}}}{V_C N_{\mathrm{A}}} = \frac{nA_{\mathrm{Mg}}}{(1.624)\left(12\sqrt{3}\right)R^3 N_{\mathrm{A}}}$$

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

$$R = \left[\frac{nA_{\mathrm{Mg}}}{(1.624)\left(12\sqrt{3}\right)\rho N_{\mathrm{A}}}\right]^{1/3}$$

$$= \left[\frac{(6 \text{ atoms/unit cell})(24.31 \text{ g/mol})}{(1.624)\left(12\sqrt{3}\right)\left(1.74 \text{ g/cm}^3\right)\left(6.023 \times 10^{23} \text{ atoms/mol}\right)}\right]^{1/3}$$

$$= 1.60 \text{ x } 10^{-8} \text{ cm} = 0.160 \text{ nm}$$

3.19 This problem asks that we calculate the unit cell volume for Co which has an HCP crystal structure. In order to do this, it is necessary to use a result of Problem 3.6, that is

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

The problem states that $c = 1.623a$, and $a = 2R$. Therefore

$$V_C = (1.623)\left(12\sqrt{3}\right)R^3$$

$$= (1.623)\left(12\sqrt{3}\right)\left(1.253 \times 10^{-8} \text{ cm}\right)^3 = 6.64 \times 10^{-23} \text{ cm}^3 = 6.64 \times 10^{-2} \text{ nm}^3$$

Crystal Systems

3.20 (a) The unit cell shown in the problem statement belongs to the tetragonal crystal system since $a = b = 0.35$ nm, $c = 0.45$ 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

$$V_C = (3.5 \times 10^{-8}\ \text{cm})^2(4.5 \times 10^{-8}\ \text{cm})$$

$$= 5.51 \times 10^{-23}\ \text{cm}^3/\text{unit cell}$$

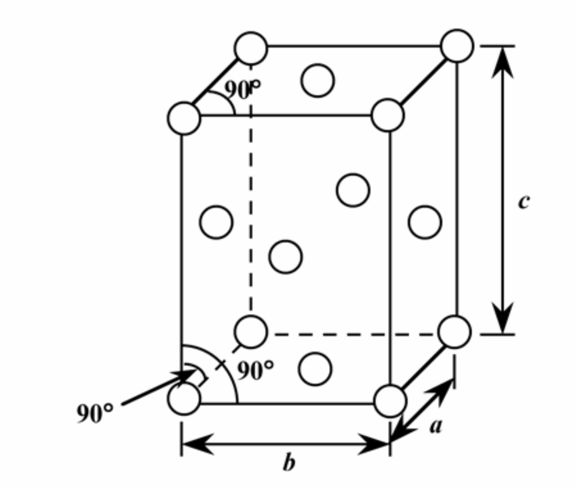
Thus, using Equation 3.5, the density is equal to

$$\rho = \frac{nA}{V_C N_\text{A}}$$

$$= \frac{(2\ \text{atoms/unit cell})(141\ \text{g/mol})}{(5.51 \times 10^{-23}\ \text{cm}^3/\text{unit cell})(6.023 \times 10^{23}\ \text{atoms/mol})}$$

$$= 8.49\ \text{g/cm}^3$$

3.21 A unit cell for the face-centered orthorhombic crystal structure is presented below.



Point Coordinates

3.22 This problem asks that we list the point coordinates for all of the atoms that are associated with the FCC unit cell. 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 $\frac{1}{2}\frac{1}{2}1$. (These coordinates are the same as bottom-face coordinates except that the “0” *z* coordinate has been replaced by a “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 Here we are asked list point coordinates for both sodium and chlorine ions for a unit cell of the sodium chloride crystal structure, which is shown in Figure 12.2.

In Figure 12.2, the chlorine ions are situated at all corners and face-centered positions. Therefore, point coordinates for these ions are the same as for FCC, as presented in the previous problem—that is, 000, 100, 110, 010, 001, 101, 111, 011, $\frac{1}{2}\frac{1}{2}0$, $\frac{1}{2}\frac{1}{2}1$, $1\frac{1}{2}\frac{1}{2}$, $0\frac{1}{2}\frac{1}{2}$, $\frac{1}{2}0\frac{1}{2}$, and $\frac{1}{2}1\frac{1}{2}$.

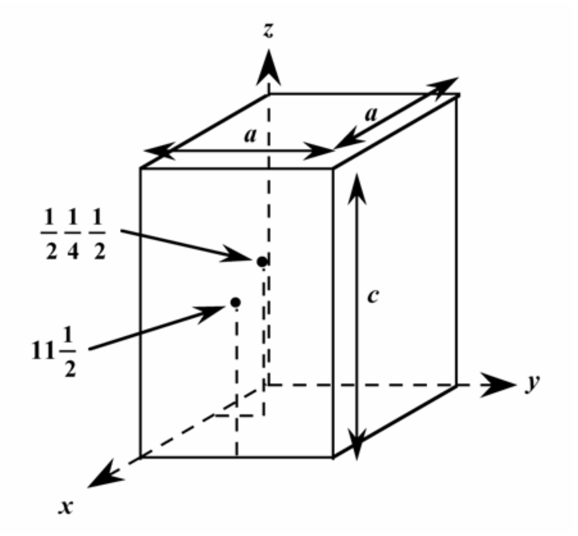
Furthermore, the sodium ions are situated at the centers of all unit cell edges, and, in addition, at the unit cell center. For the bottom face of the unit cell, the point coordinates are as follows: $\frac{1}{2}00$, $1\frac{1}{2}0$, $\frac{1}{2}10$, $0\frac{1}{2}0$. While, for the horizontal plane that passes through the center of the unit cell (which includes the ion at the unit cell center), the coordinates are $00\frac{1}{2}$, $1\,0\frac{1}{2}$, $\frac{1}{2}\frac{1}{2}\frac{1}{2}$, $1\,1\frac{1}{2}$, and $01\frac{1}{2}$. And for the four ions on the top face $\frac{1}{2}01$, $1\,\frac{1}{2}1$, $\frac{1}{2}1\,1$, and $0\frac{1}{2}1$.

3.24 This problem calls for us to list the point coordinates of both the zinc and sulfur atoms for a unit cell of the zinc blende structure, which is shown in Figure 12.4.

First of all, the sulfur atoms occupy the face-centered positions in the unit cell, which from the solution to Problem 3.22, are as follows: 000, 100, 110, 010, 001, 101, 111, 011, $\frac{1}{2}\frac{1}{2}0$, $\frac{1}{2}\frac{1}{2}1$, $1\frac{1}{2}\frac{1}{2}$, $0\frac{1}{2}\frac{1}{2}$, $\frac{1}{2}0\frac{1}{2}$, and $\frac{1}{2}1\frac{1}{2}$.

Now, using an *x-y-z* coordinate system oriented as in Figure 3.4, the coordinates of the zinc 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 zinc 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 zinc atom, located toward the upper-right-front of the unit cell, are $\frac{3}{4}\frac{3}{4}\frac{3}{4}$.

3.25 A tetragonal unit in which are shown the $1\,1\frac{1}{2}$ and $\frac{1}{2}\frac{1}{4}\frac{1}{2}$ point coordinates is presented below.



3.26 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 type, a color for the spheres (atoms), and specify an atom size. Let us enter "Sn" as the name of the atom type (since "Sn" the symbol for tin). Next it is necessary to choose a color from the selections that appear in the pull-down menu—for example, "LtBlue" (light blue). In the "Atom Size" window, it is necessary to enter an atom size. In the instructions for this step, it is suggested that the atom diameter in nanometers be used. From the table found inside the front cover of the textbook, the atomic radius for tin is 0.151 nm, and, therefore, the atomic diameter is twice this value (i.e., 0.302 nm); therefore, we enter the value "0.302". 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. Now we must enter a name in the box provided for each of the atoms in the unit cell. For example, let us name the first atom "Sn1". Its point coordinates are 000, and, therefore, we enter a "0" (zero) in each of the "x", "y", and "z" atom position boxes. Next, in the "Atom Type" pull-down menu we select "Sn", our only choice, and the name we specified in Step 1. For the next atom, which has point coordinates of 100, let us name it "Sn2"; since it is located a distance of *a* units along the *x*-axis the value of "0.583" 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 next click on the "Register" button. This same procedure is repeated for all 13 of the point coordinates specified in the problem statement. For the atom having point coordinates of "111" respective values of "0.583", "0.583", and "0.318" are entered in the x, y, and z atom position boxes, since the unit cell edge length along the *y* and *z* axes are *a* (0.583) and *c* (0.318 nm), respectively. For fractional point coordinates, the appropriate *a* or *c* value is multiplied by the fraction. For example, the second point coordinate set in the right-hand column, $\frac{1}{2}0\frac{3}{4}$, the x, y, and z atom positions are $\frac{1}{2}(0.583) = 0.2915$, 0, and $\frac{3}{4}(0.318) = 0.2385$, respectively. The x, y, and z atom position entries for all 13 sets of point coordinates are as follows:

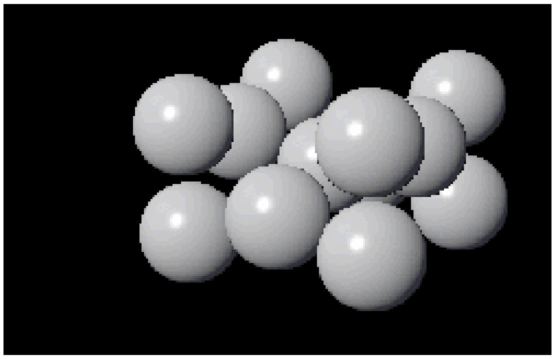
0, 0, and 0
0.583, 0, and 0
0.583, 0.583, and 0
0, 0.583, and 0
0, 0, and 0.318
0.583, 0, and 0.318
0.583, 0.583, and 0.318

0, 0.583, and 0.318
0.2915, 0, and 0.2385
0.2915, 0.583, and 0.2385
0.583, 0.2915, and 0.0795
0, 0.2915, 0.0795
0.2915, 0.2915, and 0.159

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 click on the "Go to Step 4" button). If it is decided to show bonds, probably the best thing to do is to represent unit cell edges as bonds.

The window in Step 4 presents all the data that have been entered; you may review these data for accuracy. If any changes are required, it is necessary to close out all windows back to the one in which corrections are to be made, and then reenter data in succeeding windows. When you are fully satisfied with your data, click on the "Generate" button, and the image that you have defined will be displayed. The image may then be rotated by using mouse click-and-drag.

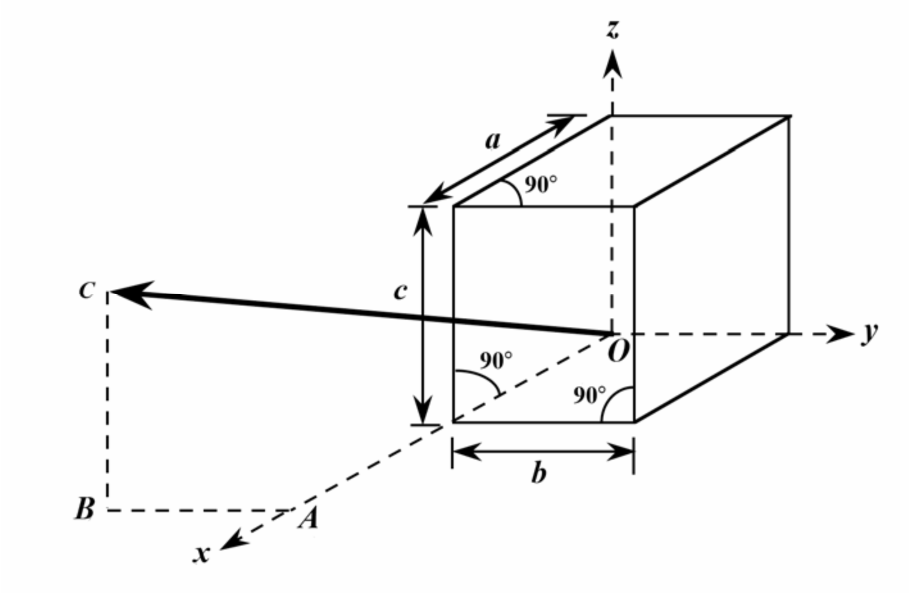
Your image should appear as



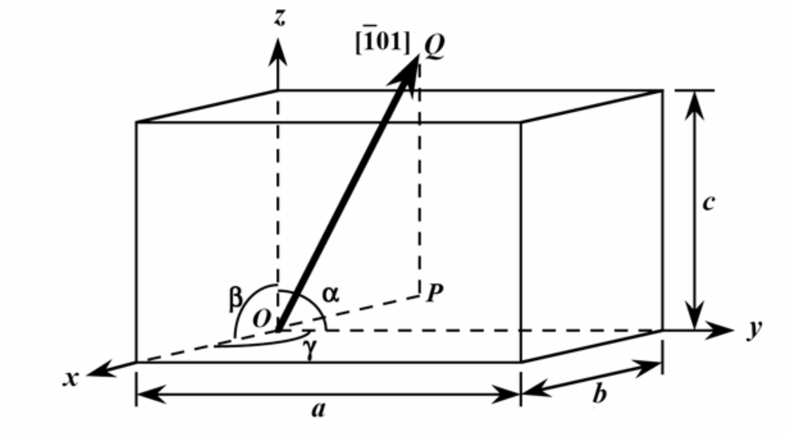
[Note: Unfortunately, with this version of the Molecular Definition Utility, it is not possible to save either the data or the image that you have generated. You may use screen capture (or screen shot) software to record and store your image.]

Crystallographic Directions

3.27 This problem calls for us to draw a $[2\bar{1}1]$ direction within an orthorhombic unit cell ($a \neq b \neq c$, $\alpha = \beta = \gamma = 90°$). Such a unit cell with its origin positioned at point *O* is shown below. We first move along the +*x*-axis 2*a* units (from point *O* to point *A*), then parallel to the +*y*-axis -*b* units (from point *A* to point *B*). Finally, we proceed parallel to the *z*-axis *c* units (from point *B* to point *C*). The $[2\bar{1}1]$ direction is the vector from the origin (point *O*) to point *C* as shown.



3.28 This problem asks that a $[\overline{1}01]$ direction be drawn within a monoclinic unit cell ($a \neq b \neq c$, and $\alpha = \beta = 90° \neq \gamma$). One such unit cell with its origin at point *O* is sketched below. For this direction, we move from the origin along the minus *x*-axis *a* units (from point *O* to point *P*). There is no projection along the *y*-axis since the next index is zero. Since the final index is a one, we move from point *P* parallel to the *z*-axis, *c* units (to point *Q*). Thus, the $[\overline{1}01]$ direction corresponds to the vector passing from the origin to point *Q*, as indicated in the figure.



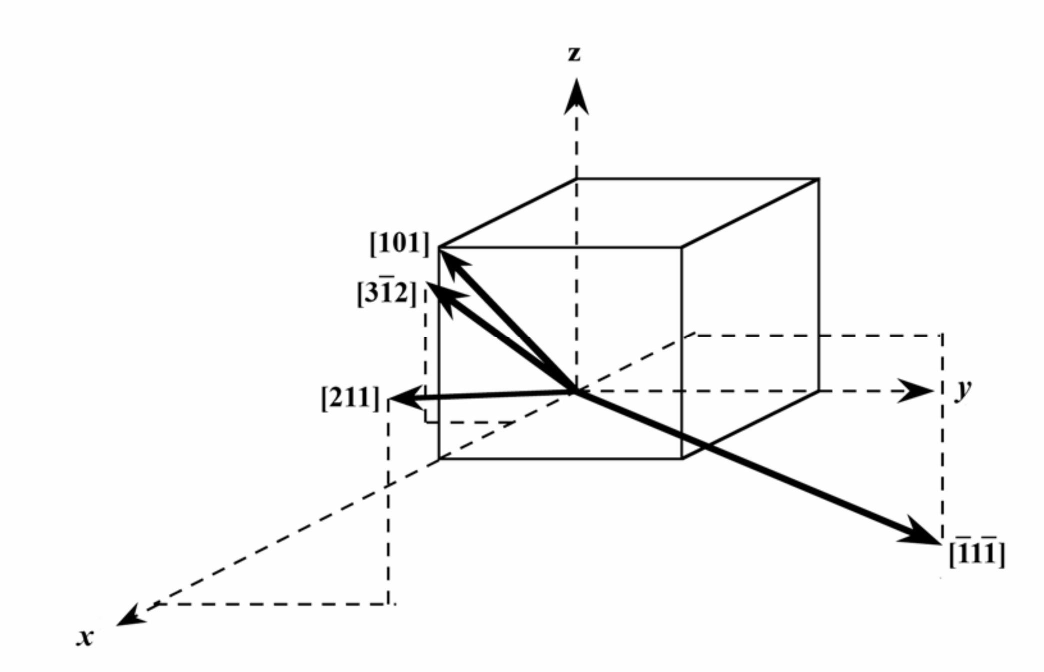
3.29 We are asked for the indices of the two directions sketched in the figure. For direction 1, the projection on the *x*-axis is *a*, while projections on the *y*- and *z*-axes are -*b*/2 and -*c*, respectively. This is a $[2\bar{1}\bar{2}]$ direction as indicated in the summary below.

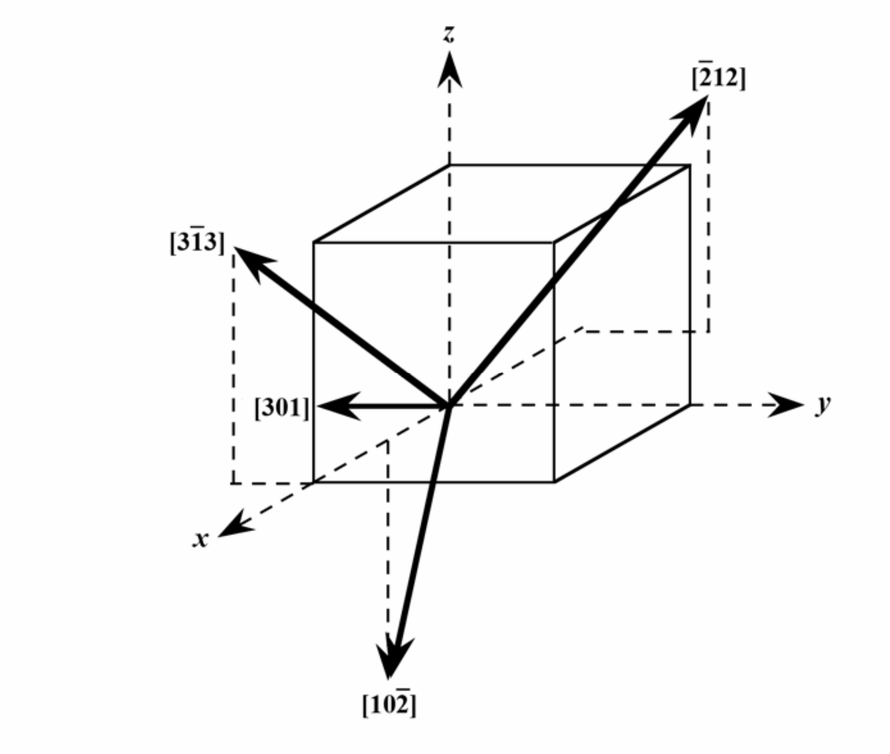
	<u>x</u>	<u>y</u>	<u>z</u>
Projections	*a*	-*b*/2	-*c*
Projections in terms of *a*, *b*, and *c*	1	-1/2	-1
Reduction to integers	2	-1	-2
Enclosure		$[2\bar{1}\bar{2}]$	

Direction 2 is [102] as summarized below.

	<u>x</u>	<u>y</u>	<u>z</u>
Projections	*a*/2	0*b*	*c*
Projections in terms of *a*, *b*, and *c*	1/2	0	1
Reduction to integers	1	0	2
Enclosure		[102]	

3.30 The directions asked for are indicated in the cubic unit cells shown below.





3.31 Direction A is a $[\bar{1}10]$ 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

	x	*y*	*z*
Projections	$-a$	b	$0c$
Projections in terms of *a*, *b*, and *c*	–1	1	0
Reduction to integers		not necessary	
Enclosure		$[\bar{1}10]$	

Direction B is a [121] direction, which determination is summarized as follows. The vector passes through the origin of the coordinate system and thus no translation is necessary. Therefore,

	x	*y*	*z*
Projections	$\frac{a}{2}$	b	$\frac{c}{2}$
Projections in terms of *a*, *b*, and *c*	$\frac{1}{2}$	1	$\frac{1}{2}$
Reduction to integers	1	2	1
Enclosure		[121]	

Direction C is a $[0\bar{1}\bar{2}]$ 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	$0a$	$-\frac{b}{2}$	$-c$
Projections in terms of *a*, *b*, and *c*	0	$-\frac{1}{2}$	–1
Reduction to integers	0	–1	–2
Enclosure		$[0\bar{1}\bar{2}]$	

Direction D is a $[1\bar{2}1]$ 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

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

3.32 Direction A is a $[33\bar{1}]$ 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	a	b	$-\frac{c}{3}$
Projections in terms of *a*, *b*, and *c*	1	1	$-\frac{1}{3}$
Reduction to integers	3	3	–1
Enclosure		$[33\bar{1}]$	

Direction B is a $[\bar{4}0\bar{3}]$ 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

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

Direction C is a $[\bar{3}61]$ 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	$-\frac{a}{2}$	b	$\frac{c}{6}$
Projections in terms of *a*, *b*, and *c*	$-\frac{1}{2}$	1	$\frac{1}{6}$
Reduction to integers	–3	6	1
Enclosure		$[\bar{3}61]$	

Direction D is a $[\bar{1}1\bar{1}]$ 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	$-\frac{a}{2}$	$\frac{b}{2}$	$-\frac{c}{2}$
Projections in terms of *a*, *b*, and *c*	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$
Reduction to integers	–1	1	–1
Enclosure		$[\bar{1}1\bar{1}]$	

3.33 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 [011] direction, equivalent directions are the following: [101], $[\bar{1}0\bar{1}]$, $[\bar{1}01]$, $[10\bar{1}]$, $[01\bar{1}]$, $[0\bar{1}1]$, and $[0\bar{1}\bar{1}]$.

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

3.34 We are asked to convert [110] and $[00\overline{1}]$ directions into the four-index Miller-Bravais scheme for hexagonal unit cells. For [110]

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

From Equations 3.6

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

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

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

$$w = w' = 0$$

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 $[uvtw] = [11\overline{2}0]$.

For $[00\overline{1}]$, $u' = 0$, $v' = 0$, and $w' = -1$; therefore,

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

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

$$t = - (0 + 0) = 0$$

$$w = -1$$

Thus, the direction is represented as $[uvtw] = [000\overline{1}]$.

3.35 This problem asks for the determination of indices for several directions in a hexagonal unit cell.

For direction A, projections on the a_1, a_2, and z axes are $-a$, $-a$, and c, or, in terms of a and c the projections are –1, –1, and 1. This means that

$u' = -1$

$v' = -1$

$w' = 1$

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

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

$$v = \frac{1}{3}(2v\tilde{O} - u\tilde{O}) = \frac{1}{3}\left[(2)(-1) - (-1)\right] = -\frac{1}{3}$$

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

$$w = w' = 1$$

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 the direction A is a $[\bar{1}\bar{1}23]$ direction.

For direction B, projections on the a_1, a_2, and z axes are $-a$, $0a$, and $0c$, or, in terms of a and c the projections are –1, 0, and 0. This means that

$u' = -1$

$v' = 0$

$w' = 0$

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

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

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

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

$$w = w' = 0$$

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 the direction B is a $[\bar{2}110]$ direction.

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

$u' = 2$

$v' = 1$

$w' = 0$

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

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

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

$$t = -(u+v) = -\left(1 - 0\right) = -1$$

$$w = w' = 0$$

No reduction is necessary inasmuch as all the indices are integers. Therefore, direction C is a $[10\bar{1}0]$.

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

$u' = 2$

$v' = 0$

$w' = 1$

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

$$u = \frac{1}{3}(2u' - v') = \frac{1}{3}\left[(2)(2) - 0\right] = \frac{4}{3}$$

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

3.36 This problem asks for us to derive expressions for each of the three primed indices in terms of the four unprimed indices.

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

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

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'*

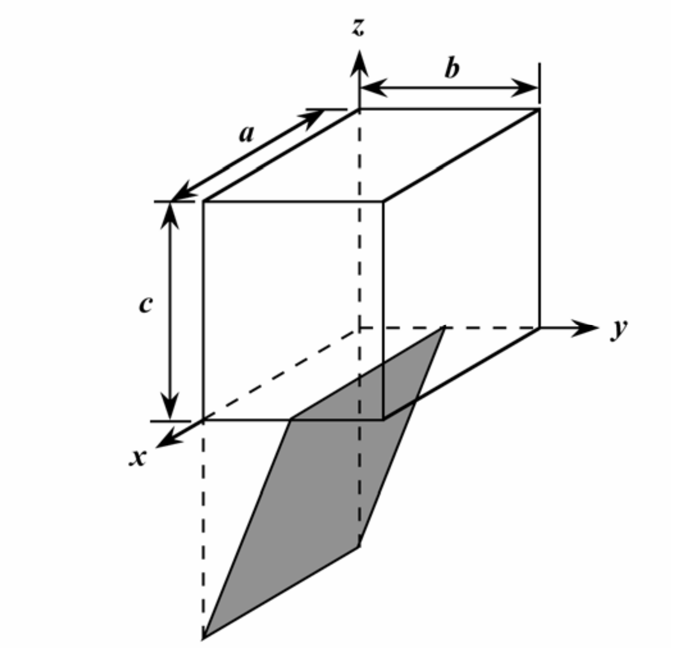
$$v' = -u - 2t = -(-v - t) - 2t = v - t$$

And, of course from Equation 3.6d

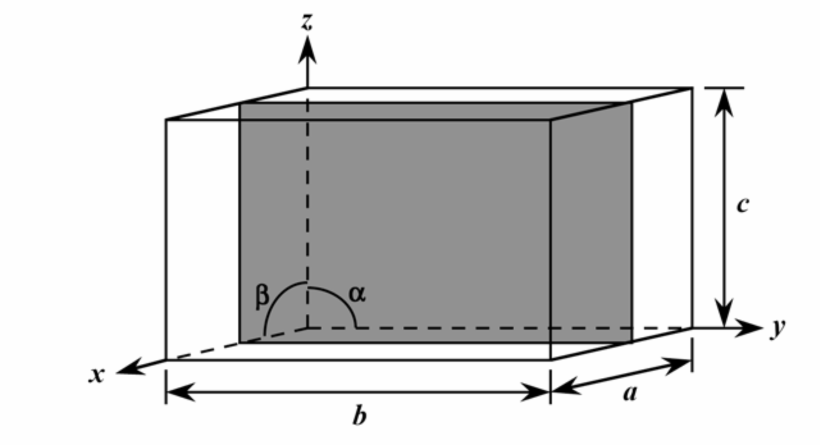
$$w' = w$$

Crystallographic Planes

3.37 (a) We are asked to draw a $(02\bar{1})$ plane within an orthorhombic unit cell. First remove the three indices from the parentheses, and take their reciprocals--i.e., ∞, 1/2, and -1. This means that the plane parallels the *x*-axis, intersects the *y*-axis at *b*/2, and intersects the *z*-axis at -*c*. 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 (200) plane is drawn within the monoclinic cell shown below. We first remove the parentheses and take the reciprocals of the indices; this gives 1/2, ∞, and ∞,. Thus, the (200) plane parallels both *y*- and *z*-axes, and intercepts the *x*-axis at *a*/2, as indicated in the drawing. (For monoclinic, $a \neq b \neq c$, and $\alpha = \gamma = 90° \neq \beta$.)



3.38 This problem calls for specification of the indices for the two planes that are drawn in the sketch.

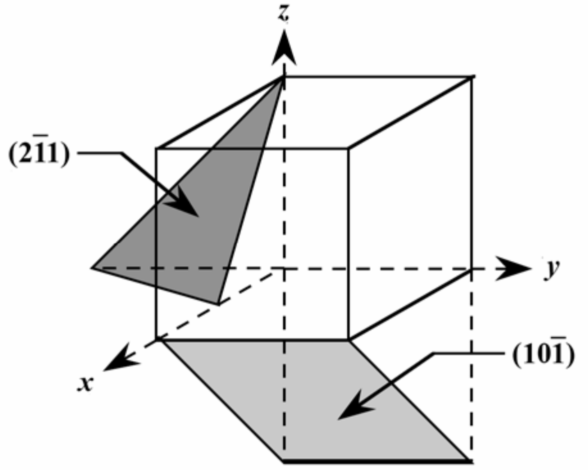
Plane 1 is a (211) plane. The determination of its indices is summarized below.

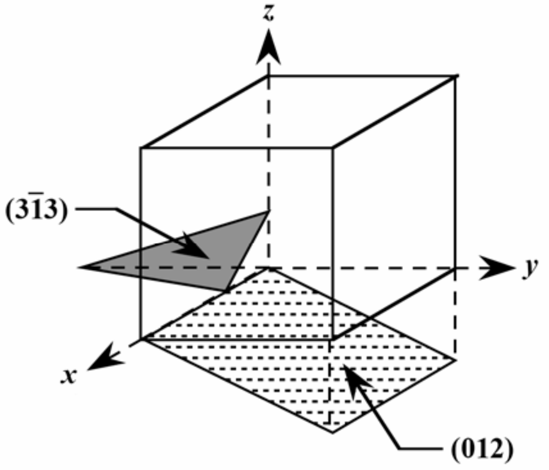
	<u>x</u>	<u>y</u>	<u>z</u>
Intercepts	*a*/2	*b*	*c*
Intercepts in terms of *a*, *b*, and *c*	1/2	1	1
Reciprocals of intercepts	2	1	1
Enclosure		(211)	

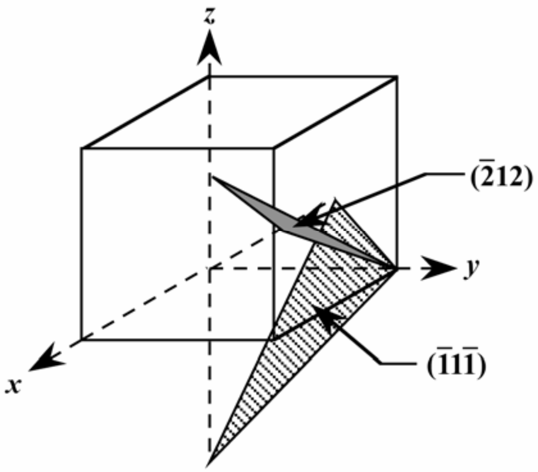
Plane 2 is a $(0\overline{2}0)$ plane, as summarized below.

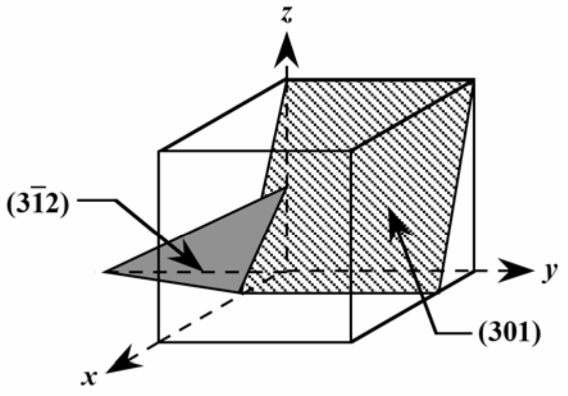
	<u>x</u>	<u>y</u>	<u>z</u>
Intercepts	∞*a*	-*b*/2	∞*c*
Intercepts in terms of *a*, *b*, and *c*	∞	-1/2	∞
Reciprocals of intercepts	0	-2	0
Enclosure		$(0\overline{2}0)$	

3.39 The planes called for are plotted in the cubic unit cells shown below.









3.40 For plane A we will leave the origin at the unit cell as shown. If we extend this plane back into the plane of the page, then it is a $(11\bar{1})$ plane, as summarized below.

	x	y	z
Intercepts	a	b	$-c$
Intercepts in terms of a, b, and c	1	1	– 1
Reciprocals of intercepts	1	1	– 1
Reduction		not necessary	
Enclosure		$(11\bar{1})$	

[*Note:* If we move the origin one unit cell distance parallel to the x axis and then one unit cell distance parallel to the y axis, the direction becomes $(\bar{1}\bar{1}1)$].

For plane B we will leave the origin of the unit cell as shown; this is a (230) plane, as summarized below.

	x	y	z
Intercepts	$\frac{a}{2}$	$\frac{b}{3}$	∞c
Intercepts in terms of a, b, and c	$\frac{1}{2}$	$\frac{1}{3}$	∞
Reciprocals of intercepts	2	3	0
Enclosure		(230)	

3.41 For plane A we will move the origin of the coordinate system one unit cell distance to the right along the y axis; thus, this is a $(1\bar{1}0)$ plane, as summarized below.

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

For plane B we will leave the origin of the unit cell as shown; thus, this is a (122) plane, as summarized below.

	$\underline{x}$	$\underline{y}$	$\underline{z}$
Intercepts	a	$\frac{b}{2}$	$\frac{c}{2}$
Intercepts in terms of a, b, and c	1	$\frac{1}{2}$	$\frac{1}{2}$
Reciprocals of intercepts	1	2	2
Reduction		not necessary	
Enclosure		(122)	

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

$$w = w' = 1$$

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 the direction D is a $[4\bar{2}\bar{2}3]$ direction.

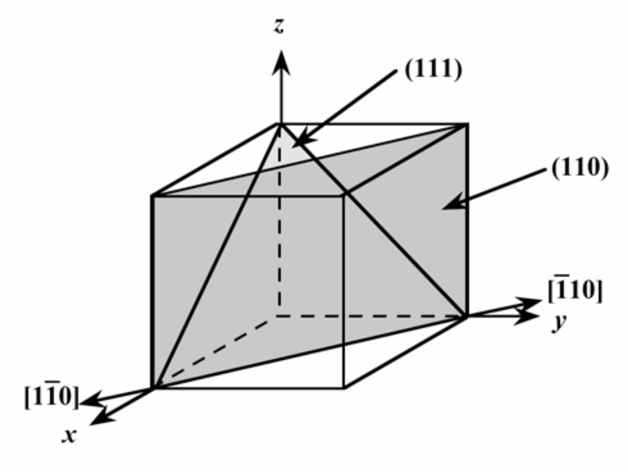
3.42 For plane A since the plane passes through the origin of the coordinate system as shown, we will move the origin of the coordinate system one unit cell distance vertically along the z axis; thus, this is a $(21\overline{1})$ plane, as summarized below.

	x	y	z
Intercepts	$\frac{a}{2}$	b	$-c$
Intercepts in terms of a, b, and c	$\frac{1}{2}$	1	– 1
Reciprocals of intercepts	2	1	– 1
Reduction		not necessary	
Enclosure		$(21\overline{1})$	

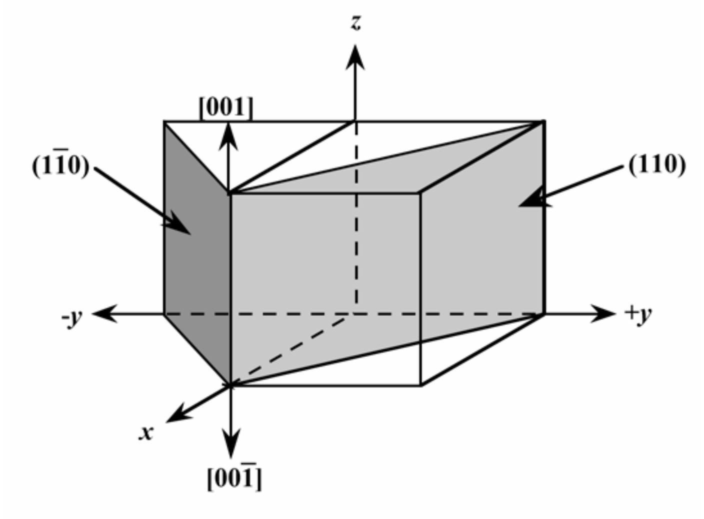
For plane B, since the plane passes through the origin of the coordinate system as shown, we will move the origin one unit cell distance vertically along the z axis; this is a $(02\overline{1})$ plane, as summarized below.

	x	y	z
Intercepts	$\infty\, a$	$\frac{b}{2}$	$-c$
Intercepts in terms of a, b, and c	∞	$\frac{1}{2}$	– 1
Reciprocals of intercepts	0	2	– 1
Reduction		not necessary	
Enclosure		$(02\overline{1})$	

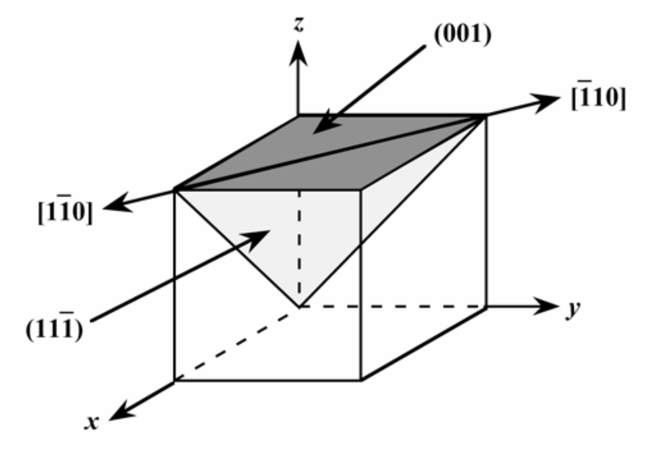
3.43 (a) In the figure below is shown (110) and (111) planes, and, as indicated, their intersection results in a $[\bar{1}10]$, or equivalently, a $[1\bar{1}0]$ direction.



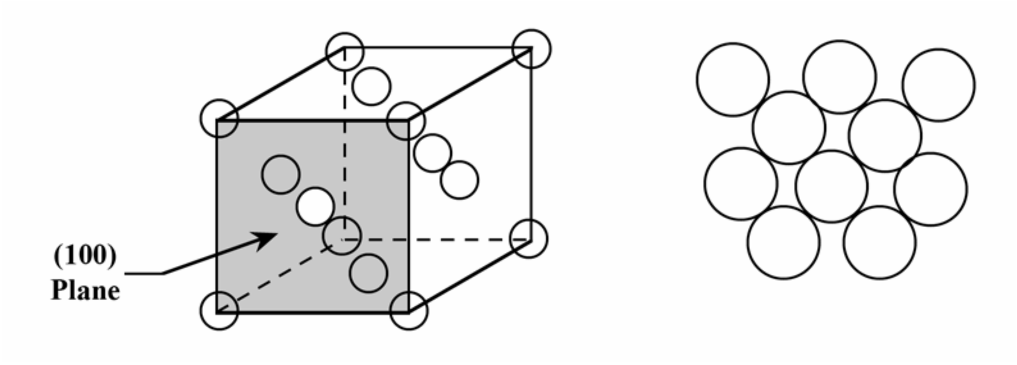
(b) In the figure below is shown (110) and $(1\bar{1}0)$ planes, and, as indicated, their intersection results in a [001], or equivalently, a $[00\bar{1}]$ direction.



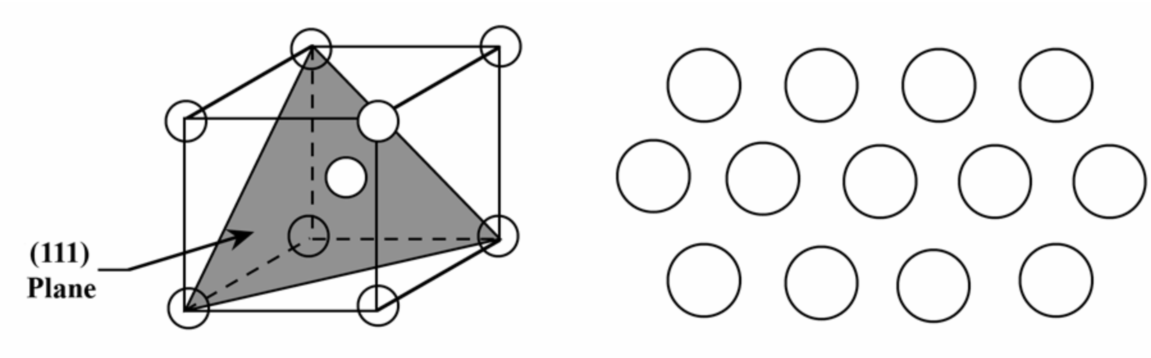
(c) In the figure below is shown $(11\bar{1})$ and (001) planes, and, as indicated, their intersection results in a $[\bar{1}10]$, or equivalently, a $[1\bar{1}0]$ direction.


z
(001)
[$\bar{1}$10]
[1$\bar{1}$0]
(11$\bar{1}$)
y
x

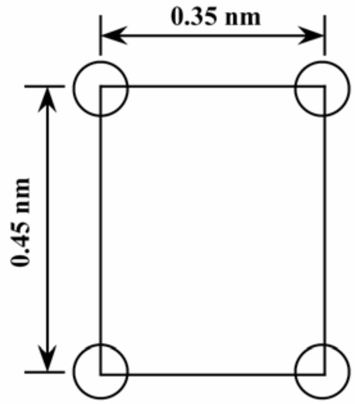
3.44 (a) The atomic packing of the (100) plane for the FCC crystal structure is called for. An FCC unit cell, its (100) plane, and the atomic packing of this plane are indicated below.



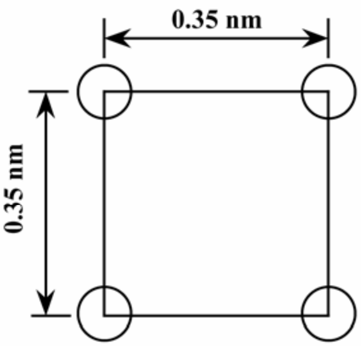
(b) For this part of the problem we are to show the atomic packing of the (111) plane for the BCC crystal structure. A BCC unit cell, its (111) plane, and the atomic packing of this plane are indicated below.



3.45 (a) The unit cell in Problem 3.20 is body-centered tetragonal. Of the three planes given in the problem statement the (100) and $(0\bar{1}0)$ are equivalent—that is, have the same atomic packing. The atomic packing for these two planes as well as the (001) are shown in the figure below.

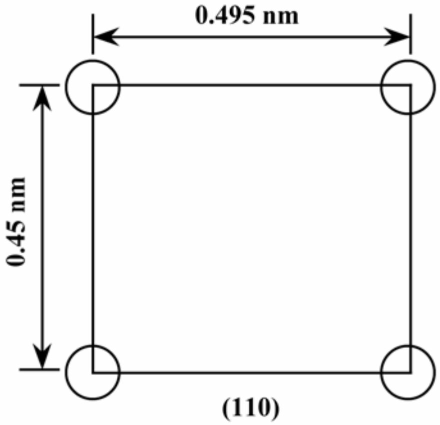


(100), $(0\bar{1}0)$

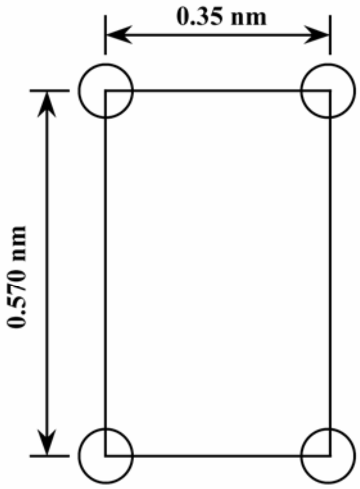


(001)

(b) Of the four planes cited in the problem statement, only (101), (011), and $(\bar{1}01)$ are equivalent—have the same atomic packing. The atomic arrangement of these planes as well as the (110) are presented in the figure below. *Note:* the 0.495 nm dimension for the (110) plane comes from the relationship $\left[(0.35\text{ nm})^2 + (0.35\text{ nm})^2\right]^{1/2}$. Likewise, the 0.570 nm dimension for the (101), (011), and $(\bar{1}01)$ planes comes from $\left[(0.35\text{ nm})^2 + (0.45\text{ nm})^2\right]^{1/2}$.

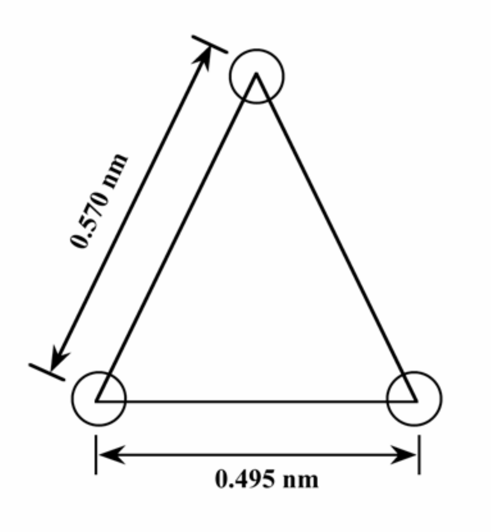


(110)

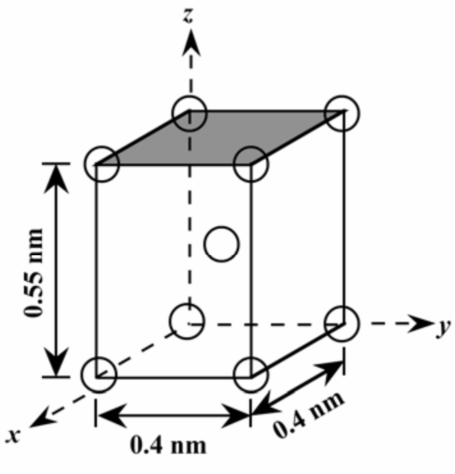


(101), (011), $(\bar{1}01)$

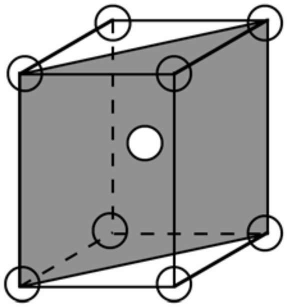
(c) All of the (111), $(1\bar{1}1)$, $(11\bar{1})$, and $(\bar{1}1\bar{1})$ planes are equivalent, that is, have the same atomic packing as illustrated in the following figure:



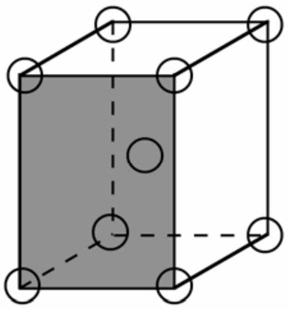
3.46 Unit cells are constructed below from the three crystallographic planes provided in the problem statement.



(001)



(110)

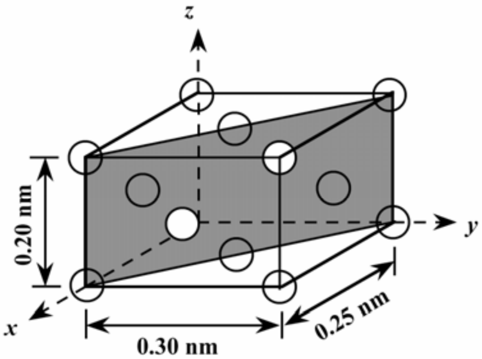


(100)

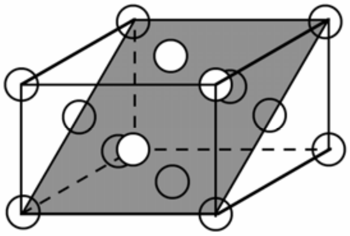
(a) This unit cell belongs to the tetragonal system since $a = b = 0.40$ nm, $c = 0.55$ nm, and $\alpha = \beta = \gamma = 90°$.

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

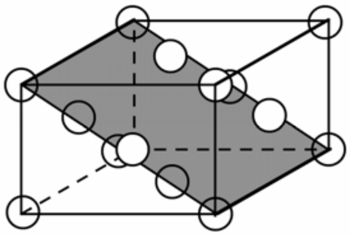
3.47 The unit cells constructed below show the three crystallographic planes that were provided in the problem statement.



(110)



(101)



(011)

(a) This unit cell belongs to the orthorhombic crystal system since a = 0.25 nm, b = 0.30 nm, c = 0.20 nm, and $\alpha = \beta = \gamma = 90°$.

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

(c) In order to compute its atomic weight, we employ Equation 3.5, with n = 4; thus

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

$$= \frac{(18.91\ \text{g/cm}^3)\ (2.0)(2.5)(3.0)\ (\times\ 10^{-24}\ \text{cm}^3\text{/unit cell})(6.023\ \times\ 10^{23}\ \text{atoms/mol})}{4\ \text{atoms/unit cell}}$$

$$= 42.7\ \text{g/mol}$$

3.48 This problem asks that we convert (111) and $(0\bar{1}2)$ planes into the four-index Miller-Bravais scheme, (*hkil*), for hexagonal cells. For (111), $h = 1$, $k = 1$, and $l = 1$, and, from Equation 3.7, the value of *i* is equal to

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

Therefore, the (111) plane becomes $(11\bar{2}1)$.

Now for the $(0\bar{1}2)$ plane, $h = 0$, $k = -1$, and $l = 2$, and computation of *i* using Equation 3.7 leads to

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

such that $(0\bar{1}2)$ becomes $(0\bar{1}12)$.

3.49 This problem asks for the determination of Bravais-Miller indices for several planes in hexagonal unit cells.

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

$h = 0$

$k = -1$

$l = 0$

Now, from Equation 3.7, the value of i is

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

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

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

$h = -1$

$k = -1$

$l = 2$

Now, from Equation 3.7, the value of i is

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

Hence, this is a $(\bar{1}\bar{1}22)$ plane.

(c) For this plane, intersections with the a_1, a_2, and z axes are $a/2$, $-a$, and ∞c (the plane parallels the z axis). In terms of a and c these intersections are 1/2, –1, and ∞, the respective reciprocals of which are 2, –1, and 0. This means that

$h = 2$

$k = -1$

$l = 0$

Now, from Equation 3.7, the value of i is

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

Hence, this is a $(2\bar{1}\bar{1}0)$ plane.

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

$h = -1$

$k = 1$

$l = 2$

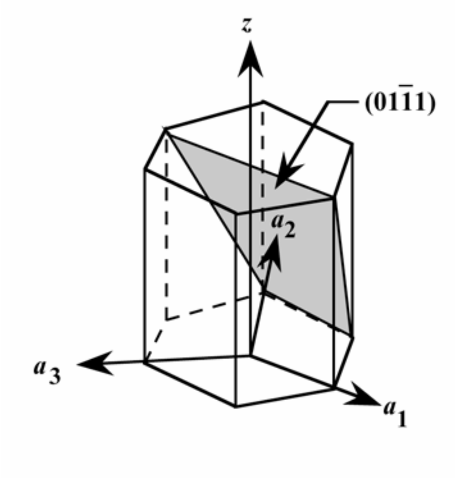
Now, from Equation 3.7, the value of i is

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

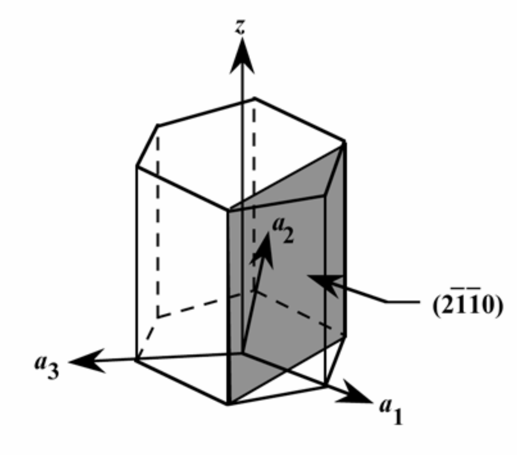
Therefore, this is a $(\bar{1}102)$ plane.

3.50 This problem asks that we draw $(01\bar{1}1)$ and $(2\bar{1}\bar{1}0)$ planes within hexagonal unit cells.

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

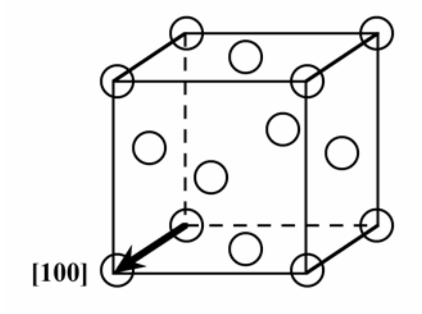


For $(2\bar{1}\bar{1}0)$ the reciprocals of h, k, i, and l are, respectively, 1/2, –1, –1, and ∞; thus, this plane is parallel to the c axis, and intersects the a_1 axis at $a/2$, the a_2 axis at $-a$, and the a_3 axis at $-a$. The plane having these intersections is shown in the figure below.



Linear and Planar Densities

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

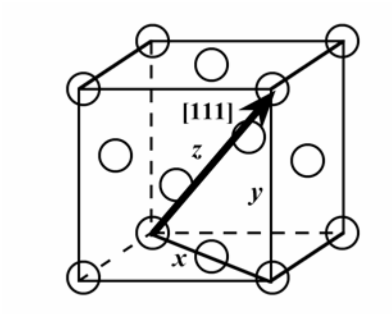


For this [100] direction there is one atom at each of the two unit cell corners, and, thus, there is the equivalent of 1 atom that is centered on the direction vector. The length of this direction vector is just the unit cell edge length, $2R\sqrt{2}$ (Equation 3.1). Therefore, the expression for the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

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

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

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:

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

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

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

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

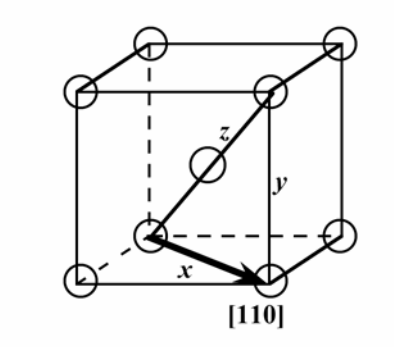
(b) From the table inside the front cover, the atomic radius for copper is 0.128 nm. Therefore, the linear density for the [100] direction is

$$\mathrm{LD}_{100}(\mathrm{Cu}) = \frac{1}{2R\sqrt{2}} = \frac{1}{(2)(0.128 \text{ nm})\sqrt{2}} = 2.76 \text{ nm}^{-1} = 2.76 \times 10^9 \text{ m}^{-1}$$

While for the [111] direction

$$\mathrm{LD}_{111}(\mathrm{Cu}) = \frac{1}{2R\sqrt{6}} = \frac{1}{(2)(0.128 \text{ nm})\sqrt{6}} = 1.59 \text{ nm}^{-1} = 1.59 \times 10^9 \text{ m}^{-1}$$

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



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 $\frac{4R}{\sqrt{3}}$. 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:

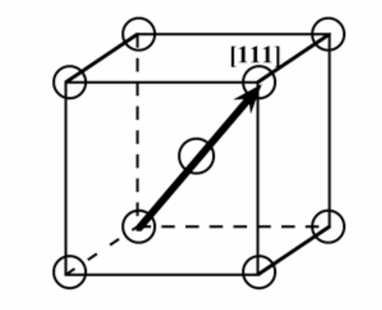
$$x = \sqrt{(4R)^2 - \left(\frac{4R}{\sqrt{3}}\right)^2} = \sqrt{\frac{32R^2}{3}} = 4R\sqrt{\frac{2}{3}}$$

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

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

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

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 4*R*, since all of the atoms whose centers the vector passes through touch one another. Therefore, the linear density is equal to

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

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

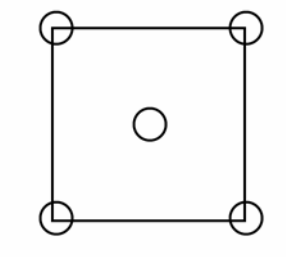
(b) From the table inside the front cover, the atomic radius for iron is 0.124 nm. Therefore, the linear density for the [110] direction is

$$\mathrm{LD}_{110}(\mathrm{Fe}) = \frac{\sqrt{3}}{4R\sqrt{2}} = \frac{\sqrt{3}}{(4)(0.124 \text{ nm})\sqrt{2}} = 2.47 \text{ nm}^{-1} = 2.47 \times 10^{9} \text{ m}^{-1}$$

While for the [111] direction

$$\mathrm{LD}_{111}(\mathrm{Fe}) = \frac{1}{2R} = \frac{1}{(2)(0.124 \text{ nm})} = 4.03 \text{ nm}^{-1} = 4.03 \times 10^{9} \text{ m}^{-1}$$

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

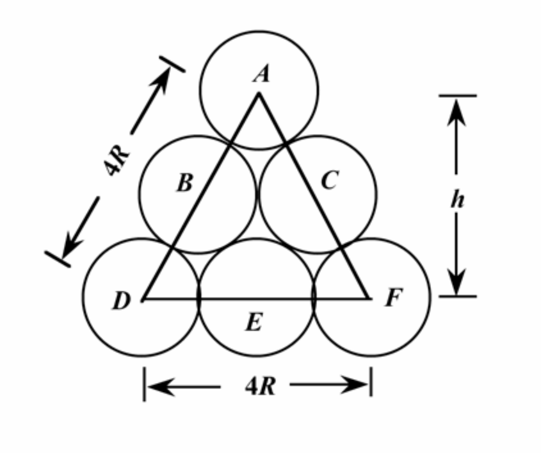


For this (100) plane there is one atom at each of the four cube corners, each of which is shared with four adjacent unit cells, while the center atom lies entirely within the unit cell. Thus, there is the equivalence of 2 atoms associated with this FCC (100) plane. The planar section represented in the 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

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

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

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

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

And, thus, the planar density is

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

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

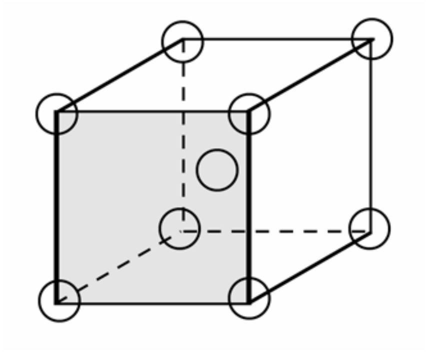
(b) From the table inside the front cover, the atomic radius for aluminum is 0.143 nm. Therefore, the planar density for the (100) plane is

$$\text{PD}_{100}(\text{Al}) = \frac{1}{4R^2} = \frac{1}{4(0.143 \text{ nm})^2} = 12.23 \text{ nm}^{-2} = 1.223 \times 10^{19} \text{ m}^{-2}$$

While for the (111) plane

$$\text{PD}_{111}(\text{Al}) = \frac{1}{2R^2\sqrt{3}} = \frac{1}{2\sqrt{3}(0.143 \text{ nm})^2} = 14.12 \text{ nm}^{-2} = 1.412 \times 10^{19} \text{ m}^{-2}$$

3.54 (a) A BCC unit cell within which is drawn a (100) plane is shown below.

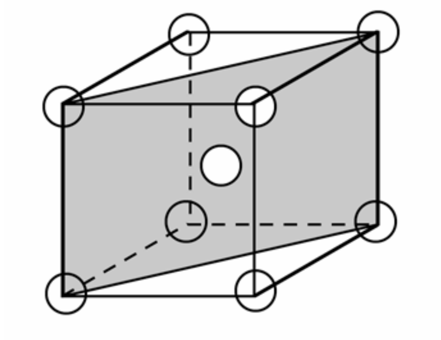


For this (100) plane there is one atom at each of the four cube corners, each of which is shared with four adjacent unit cells. Thus, there is the equivalence of 1 atom associated with this BCC (100) plane. The planar section represented in the above figure is a square, wherein the side lengths are equal to the unit cell edge length, $\frac{4R}{\sqrt{3}}$ (Equation 3.3); and, thus, the area of this square is just $\left(\frac{4R}{\sqrt{3}}\right)^2 = \frac{16R^2}{3}$. Hence, the planar density for this (100) plane is just

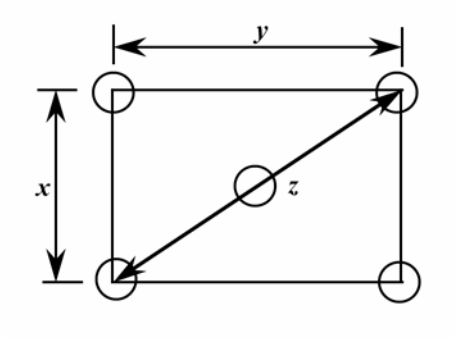
$$\mathrm{PD}_{100} = \frac{\text{number of atoms centered on (100) plane}}{\text{area of (100) plane}}$$

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

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 $\frac{4R}{\sqrt{3}}$. Now, the diagonal length *z* is equal to 4*R*. 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

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

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

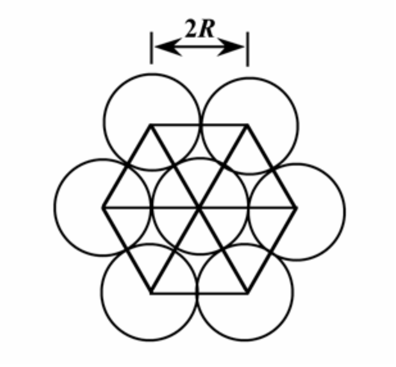
(b) From the table inside the front cover, the atomic radius for molybdenum is 0.136 nm. Therefore, the planar density for the (100) plane is

$$\mathrm{PD}_{100}(\mathrm{Mo}) = \frac{3}{16R^2} = \frac{3}{16(0.136\ \mathrm{nm})^2} = 10.14\ \mathrm{nm}^{-2} = 1.014 \times 10^{19}\ \mathrm{m}^{-2}$$

While for the (110) plane

$$\mathrm{PD}_{110}(\mathrm{Mo}) = \frac{3}{8R^2\sqrt{2}} = \frac{3}{8(0.136\ \mathrm{nm})^2\sqrt{2}} = 14.34\ \mathrm{nm}^{-2} = 1.434 \times 10^{19}\ \mathrm{m}^{-2}$$

3.55 (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

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

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

(b) From the table inside the front cover, the atomic radius for titanium is 0.145 nm. Therefore, the planar density for the (0001) plane is

$$\mathrm{PD}_{0001}(\mathrm{Ti}) = \frac{1}{2R^2\sqrt{3}} = \frac{1}{2\sqrt{3}\,(0.145 \text{ nm})^2} = 13.73 \text{ nm}^{-2} = 1.373 \times 10^{19} \text{ m}^{-2}$$

Polycrystalline Materials

3.56 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

3.57 From the Table 3.1, 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

$$a = 2R\sqrt{2} = (2)(0.1431\ \text{nm})\sqrt{2} = 0.4048\ \text{nm}$$

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

$$d_{110} = \frac{a}{\sqrt{(1)^2 + (1)^2 + (0)^2}} = \frac{0.4048\ \text{nm}}{\sqrt{2}} = 0.2862\ \text{nm}$$

3.58 We first calculate the lattice parameter using Equation 3.3 and the value of *R* (0.1249 nm) cited in Table 3.1, as follows:

$$a = \frac{4R}{\sqrt{3}} = \frac{(4)(0.1249 \text{ nm})}{\sqrt{3}} = 0.2884 \text{ nm}$$

Next, the interplanar spacing for the (310) set of planes may be determined using Equation 3.14 according to

$$d_{310} = \frac{a}{\sqrt{(3)^2 + (1)^2 + (0)^2}} = \frac{0.2884 \text{ nm}}{\sqrt{10}} = 0.0912 \text{ nm}$$

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

$$\sin \theta = \frac{n\lambda}{2d_{310}} = \frac{(1)(0.0711 \text{ nm})}{(2)(0.0912 \text{ nm})} = 0.390$$

Which leads to

$$\theta = \sin^{-1}(0.390) = 22.94°$$

And, finally

$$2\theta = (2)(22.94°) = 45.88°$$

3.59 From the table, α-iron has a BCC crystal structure and an atomic radius of 0.1241 nm. Using Equation 3.3 the lattice parameter, *a*, may be computed as follows:

$$a = \frac{4R}{\sqrt{3}} = \frac{(4)(0.1241 \text{ nm})}{\sqrt{3}} = 0.2866 \text{ nm}$$

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

$$d_{111} = \frac{a}{\sqrt{(1)^2 + (1)^2 + (1)^2}} = \frac{0.2866 \text{ nm}}{\sqrt{3}} = 0.1655 \text{ nm}$$

And, similarly for d_{211}

$$d_{211} = \frac{a}{\sqrt{(2)^2 + (1)^2 + (1)^2}} = \frac{0.2866 \text{ nm}}{\sqrt{6}} = 0.1170 \text{ nm}$$

3.60 (a) From the data given in the problem, and realizing that 36.12° = 2θ, the interplanar spacing for the (311) set of planes for rhodium may be computed using Equation 3.13 as

$$d_{311} = \frac{n\lambda}{2\sin\theta} = \frac{(1)(0.0711 \text{ nm})}{(2)\left(\sin \frac{36.12°}{2}\right)} = 0.1147 \text{ nm}$$

(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 Rh has an FCC crystal structure. Therefore,

$$a = d_{311}\sqrt{(3)^2 + (1)^2 + (1)^2} = (0.1147 \text{ nm})\left(\sqrt{11}\right) = 0.3804 \text{ nm}$$

And, from Equation 3.1

$$R = \frac{a}{2\sqrt{2}} = \frac{0.3804 \text{ nm}}{2\sqrt{2}} = 0.1345 \text{ nm}$$

3.61 (a) From the data given in the problem, and realizing that 75.99° = 2θ, the interplanar spacing for the (211) set of planes for Nb may be computed using Equation 3.13 as follows:

$$d_{211} = \frac{n\lambda}{2\sin\theta} = \frac{(1)(0.1659\ \text{nm})}{(2)\left(\sin\dfrac{75.99°}{2}\right)} = 0.1348\ \text{nm}$$

(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 Nb has a BCC crystal structure. Therefore,

$$a = d_{211}\sqrt{(2)^2 + (1)^2 + (1)^2} = (0.1347\ \text{nm})\left(\sqrt{6}\right) = 0.3300\ \text{nm}$$

And, from Equation 3.3

$$R = \frac{a\sqrt{3}}{4} = \frac{(0.3300\ \text{nm})\sqrt{3}}{4} = 0.1429\ \text{nm}$$

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

$$d_{hkl} = \frac{n\lambda}{2\sin\theta} = \frac{(1)(0.1542\ \text{nm})}{(2)\left(\sin\dfrac{44.53°}{2}\right)} = 0.2035\ \text{nm}$$

Now, employment of both Equations 3.14 and 3.1 (since Ni's crystal structure is FCC), and the value of R for nickel from Table 3.1 (0.1246 nm) leads to

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

$$= \frac{(2)(0.1246\ \text{nm})\sqrt{2}}{(0.2035\ \text{nm})} = 1.732$$

This means that

$$h^2 + k^2 + l^2 = (1.732)^2 = 3.0$$

By trial and error, the only three integers that are all odd or even, the sum of the squares of which equals 3.0 are 1, 1, and 1. Therefore, the set of planes responsible for this diffraction peak is the (111) set.

3.63 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 3.21, which results from diffraction by the (111) set of planes, occurs at 2θ = 31.3°; the corresponding interplanar spacing for this set of planes, using Equation 3.13, is equal to

$$d_{111} = \frac{n\lambda}{2 \sin \theta} = \frac{(1)(0.1542 \text{ nm})}{(2)\left(\sin \dfrac{31.3°}{2}\right)} = 0.2858 \text{ nm}$$

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

$$a = d_{hkl}\sqrt{(h)^2 + (k)^2 + (l)^2} = d_{111}\sqrt{(1)^2 + (1)^2 + (1)^2}$$

$$= (0.2858 \text{ nm})\sqrt{3} = 0.4950 \text{ nm}$$

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

Peak Index	2θ	d_{hkl}(nm)	*a* (nm)
200	36.6	0.2455	0.4910
220	52.6	0.1740	0.4921
311	62.5	0.1486	0.4929
222	65.5	0.1425	0.4936

3.64 The first four diffraction peaks that will occur for BCC consistent with $h + k + l$ being even are (110), (200), (211), and (220).

3.65 (a) Since W has a BCC crystal structure, only those peaks for which $h + k + l$ are even will appear. Therefore, the first peak results by diffraction from (110) 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 40.2°

$$d_{110} = \frac{n\lambda}{2 \sin \theta} = \frac{(1)(0.1542 \text{ nm})}{(2)\left(\sin \frac{40.2°}{2}\right)} = 0.2244 \text{ nm}$$

(c) Employment of Equations 3.14 and 3.3 is necessary for the computation of R for W as

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

$$= \frac{(0.2244 \text{ nm})(\sqrt{3})\sqrt{(1)^2 + (1)^2 + (0)^2}}{4}$$

$$= 0.1374 \text{ nm}$$

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

Peak Index	2θ	d_{hkl}(nm)	R (nm)
200	58.4	0.1580	0.1369
211	73.3	0.1292	0.1370
220	87.0	0.1120	0.1371
310	100.7	0.1001	0.1371

Noncrystalline Solids

3.66 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.