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

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

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

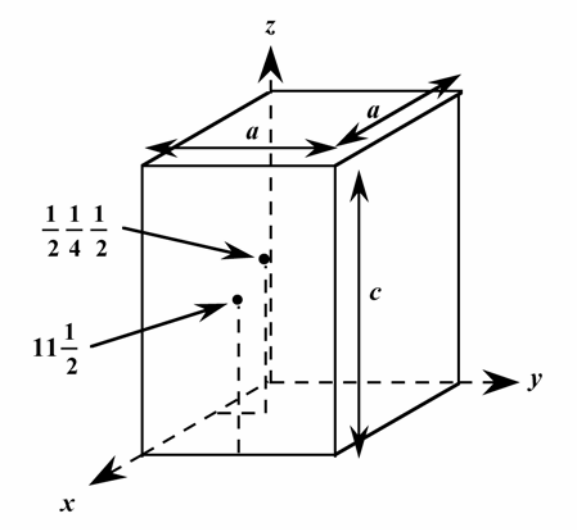
Thus, using Equation 3.5, the density is equal to

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

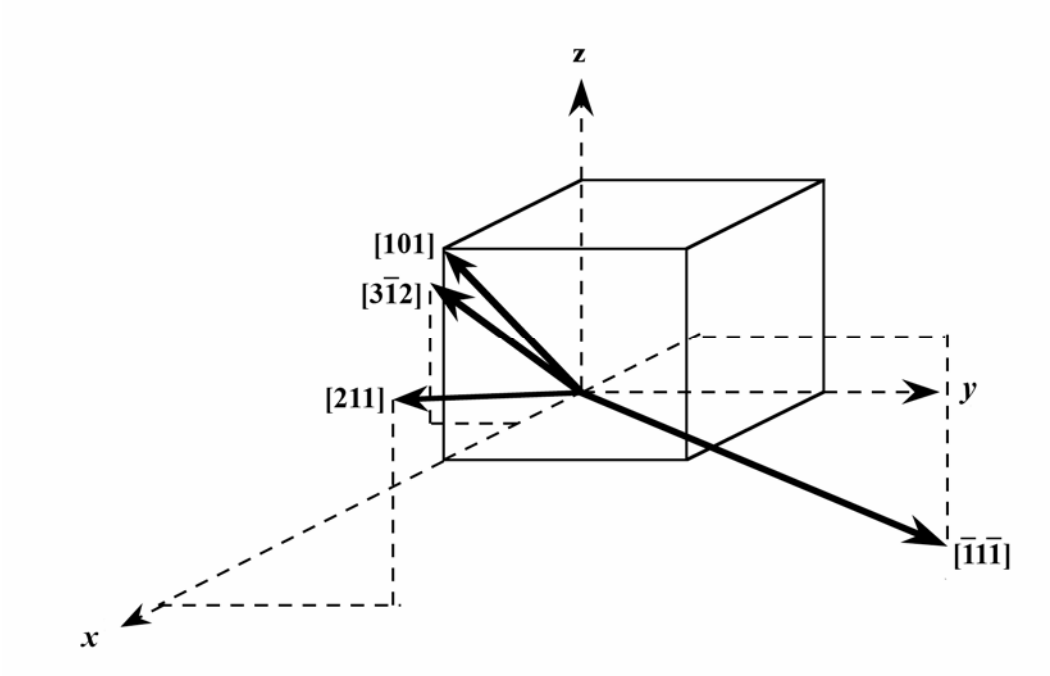
$$= \frac{(2\ \text{atoms/unit cell})(141\ \text{g/mol})}{(5.51 \times 10^{-23}\ \text{cm}^3/\text{unit cell})(6.023 \times 10^{23}\ \text{atoms/mol})}$$

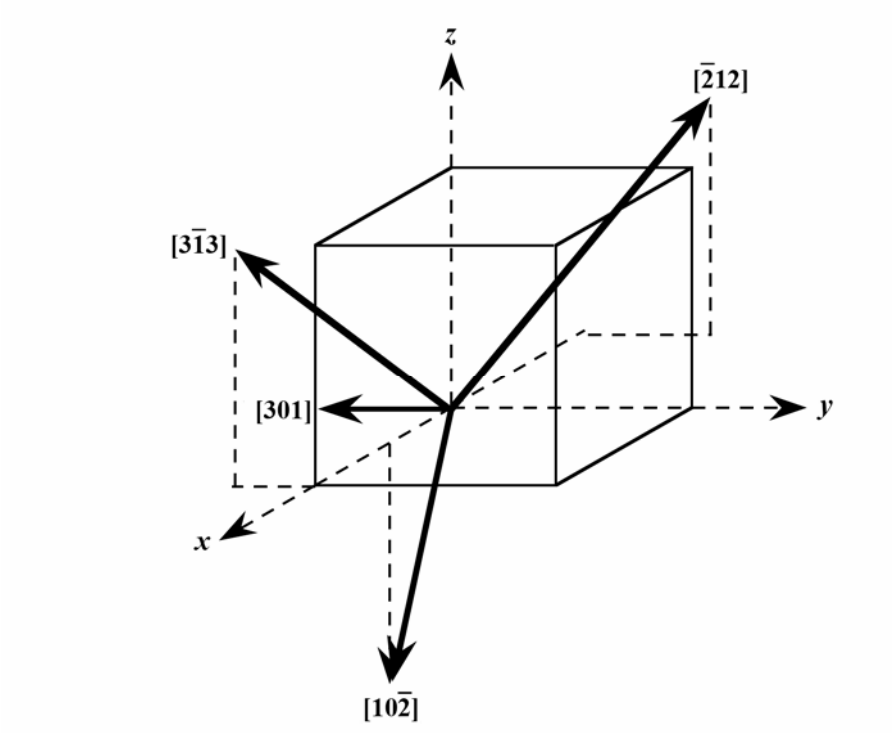
$$= 8.49\ \text{g/cm}^3$$

3.25 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.



3.30 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

	x	y	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

	x	y	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

	x	y	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

	x	y	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		$[\bar{1}1\bar{1}]$	

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

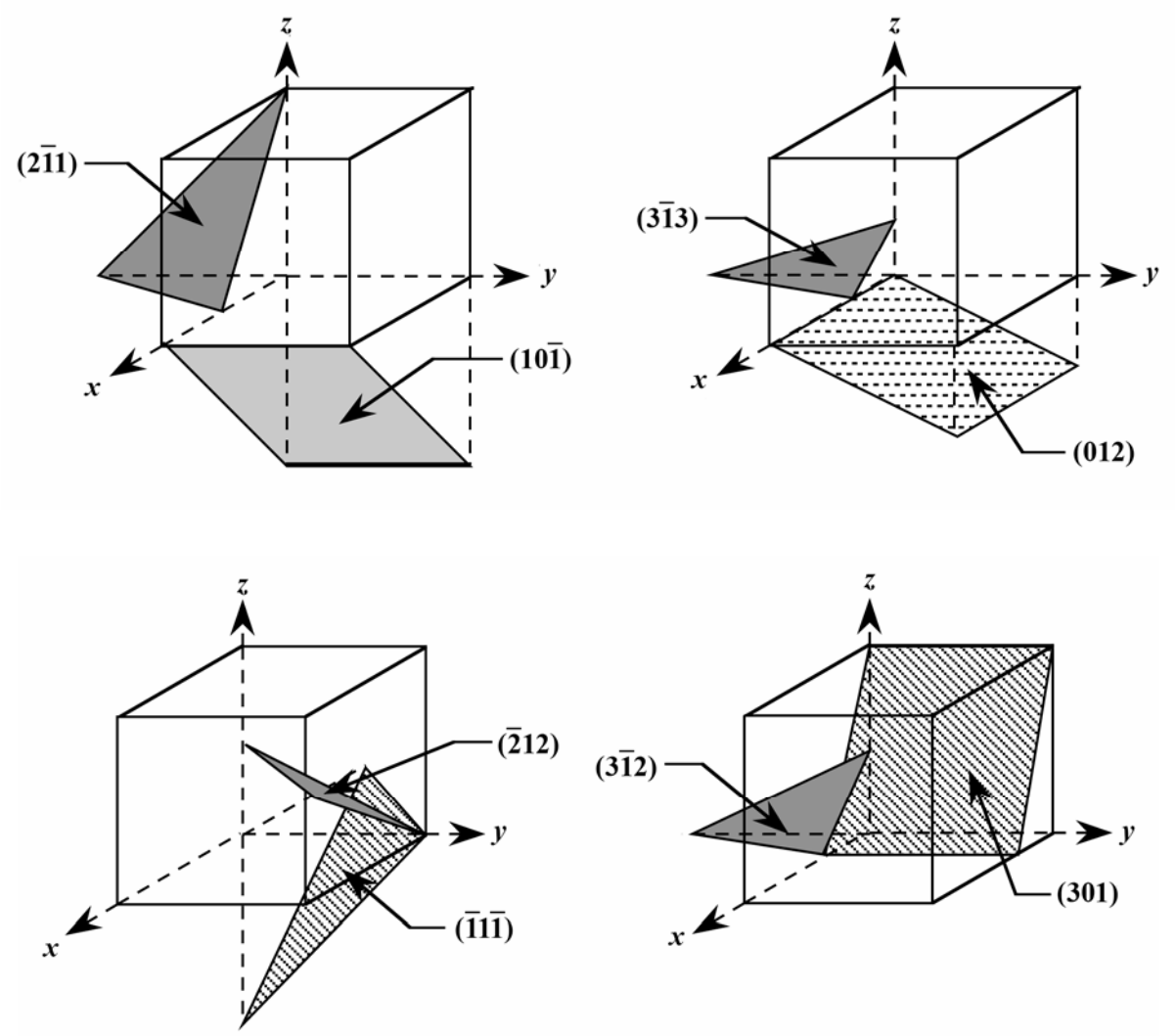
Plane 1 is a (211) plane. The determination of its indices is summarized below.

	x	y	z
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 $(0\bar{2}0)$ plane, as 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		$(0\bar{2}0)$	

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.

	x	y	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.

	x	y	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)	

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

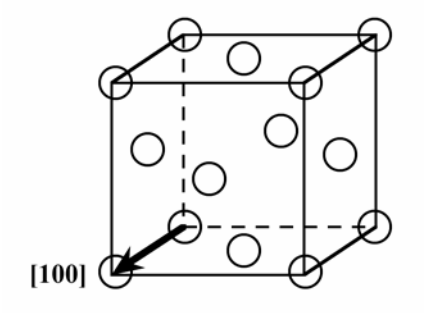
$$h = 2$$
$$k = -1$$
$$l = 0$$

Now, from Equation 3.7, the value of i is

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

Linear and Planar Densities

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

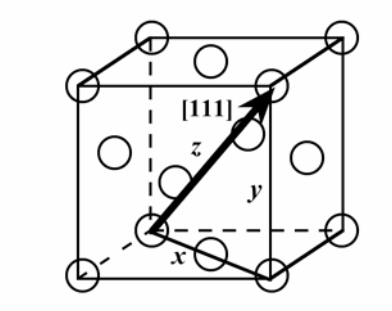


For this [100] direction there is one atom at each of the two unit cell corners, and, thus, there is the equivalent of 1 atom that is centered on the direction vector. The length of this direction vector is just the unit cell edge length, $2R\sqrt{2}$ (Equation 3.1). Therefore, the expression for the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

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

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

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

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

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

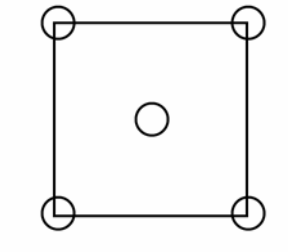
(b) From the table inside the front cover, the atomic radius for copper is 0.128 nm. Therefore, the linear density for the [100] direction is

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

While for the [111] direction

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

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

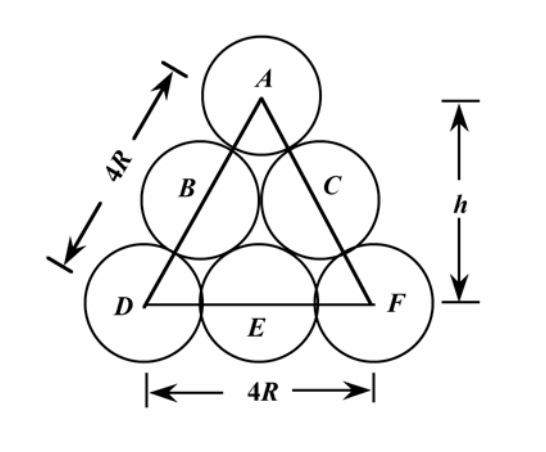


For this (100) plane there is one atom at each of the four cube corners, each of which is shared with four adjacent unit cells, while the center atom lies entirely within the unit cell. Thus, there is the equivalence of 2 atoms associated with this FCC (100) plane. The planar section represented in the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

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

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

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

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

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}

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

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

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

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.

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