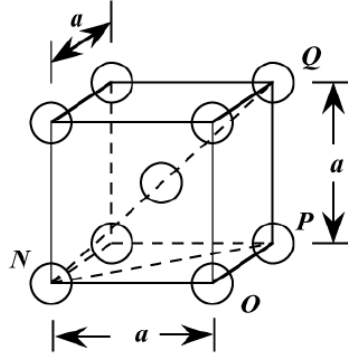


HW#2
Due Jan 29

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

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

3.10 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, $a = 2R$. Therefore, employment of Equation 3.5 yields

$$\begin{aligned} \rho &= \frac{nA}{V_C N_A} = \frac{nA}{(2R)^3 N_A} \\ &= \frac{(1 \text{ atom/unit cell})(74.5 \text{ g/mol})}{\left\{ \left[(2)(1.45 \times 10^{-8} \text{ cm}) \right]^3 / (\text{unit cell}) \right\} (6.023 \times 10^{23} \text{ atoms/mol})} \\ &= 5.07 \text{ g/cm}^3 \end{aligned}$$

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

$$\begin{aligned} n &= \frac{(\text{APF}) a^2 c}{\frac{4}{3} \pi R^3} \\ &= \frac{(0.693)(4.59)^2 (4.95) (10^{-24} \text{ cm}^3)}{\frac{4}{3} \pi (1.625 \times 10^{-8} \text{ cm})^3} \\ &= 4.0 \text{ atoms/unit cell} \end{aligned}$$

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

$$\begin{aligned} \rho &= \frac{n A_{\text{In}}}{a^2 c N_A} \\ &= \frac{(4 \text{ atoms/unit cell})(114.82 \text{ g/mol})}{\left[(4.59 \times 10^{-8} \text{ cm})^2 (4.95 \times 10^{-8} \text{ cm})/\text{unit cell} \right] (6.023 \times 10^{23} \text{ atoms/mol})} \\ &= 7.31 \text{ g/cm}^3 \end{aligned}$$

3.30 (a) This part of the problem calls for us to determine the unit cell edge length for MgO. The density of MgO is 3.58 g/cm^3 and the crystal structure is rock salt. From Equation 3.6

$$\rho = \frac{n(A_{\text{Mg}} + A_{\text{O}})}{V_C N_A} = \frac{n(A_{\text{Mg}} + A_{\text{O}})}{a^3 N_A}$$

Or, solving for a

$$\begin{aligned} a &= \left[\frac{n(A_{\text{Mg}} + A_{\text{O}})}{\rho N_A} \right]^{1/3} \\ &= \left[\frac{(4 \text{ formula units/unit cell})(24.31 \text{ g/mol} + 16.00 \text{ g/mol})}{(3.58 \text{ g/cm}^3)(6.023 \times 10^{23} \text{ formula units/mol})} \right]^{1/3} \\ &= 4.21 \times 10^{-8} \text{ cm} = 0.421 \text{ nm} \end{aligned}$$

(b) The edge length is determined from the Mg^{2+} and O^{2-} radii for this portion of the problem. Now

$$a = 2r_{\text{Mg}^{2+}} + 2r_{\text{O}^{2-}}$$

From Table 3.4

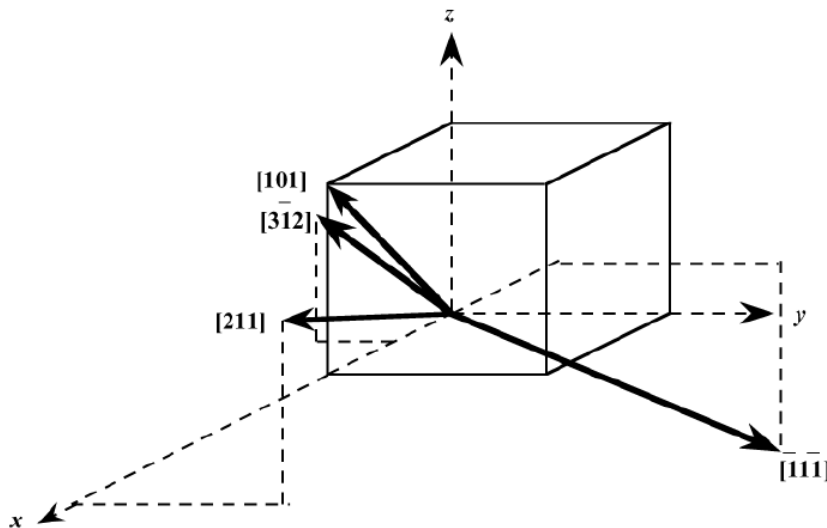
$$a = 2(0.072 \text{ nm}) + 2(0.140 \text{ nm}) = 0.424 \text{ nm}$$

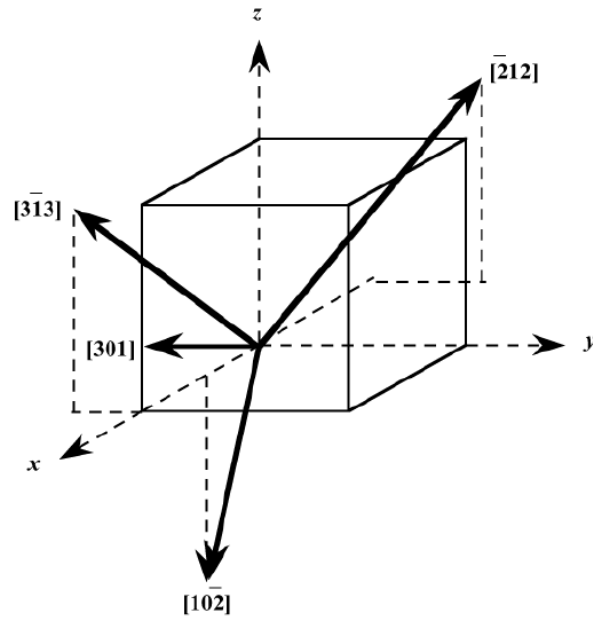
3.43 This problem asks that we list the point coordinates for all of the atoms that are associated with the FCC unit cell. From Figure 3.1b, the atom located at the origin of the unit cell has the coordinates 000. Coordinates for other atoms in the bottom face are 100, 110, 010, and $\frac{1}{2}\frac{1}{2}0$. (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 $\frac{1}{2}1\frac{1}{2}$.

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





3.52 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	$[121]$		

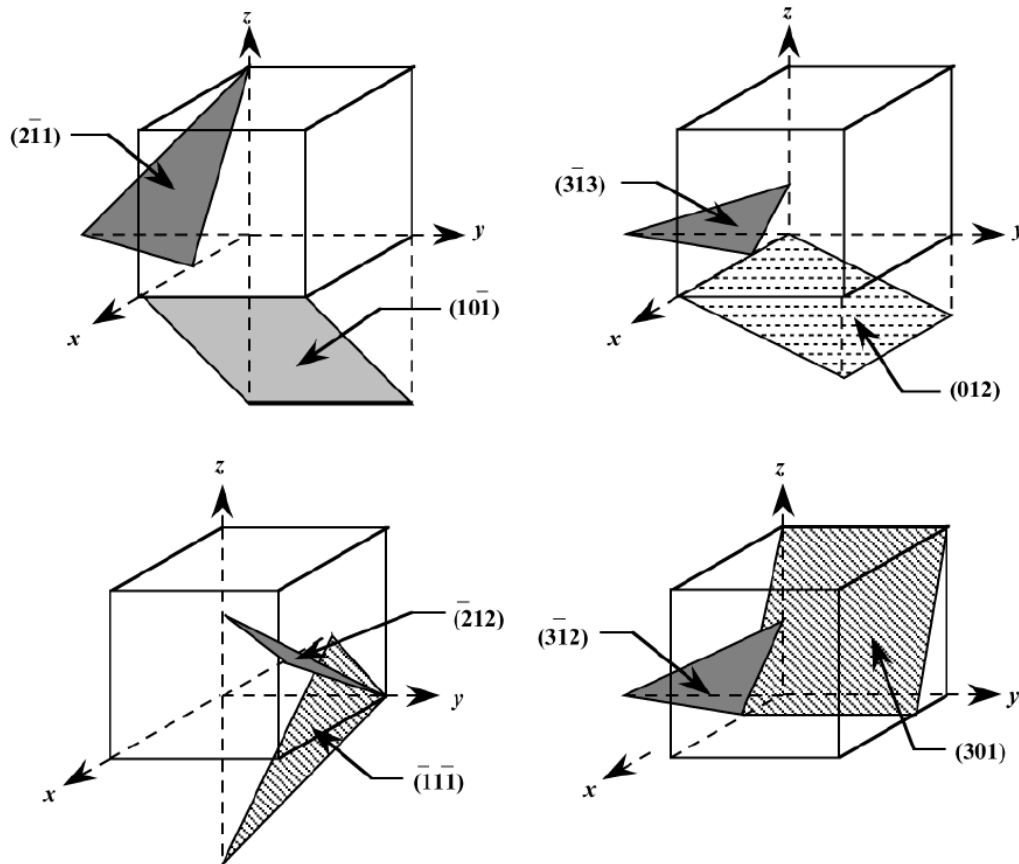
Direction C is a $[0\bar{1}\bar{2}]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	\underline{x}	\underline{y}	\underline{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

	\underline{x}	\underline{y}	\underline{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		$[1\bar{2}1]$	

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



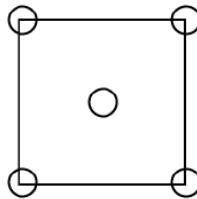
3.62 For plane A we will move the origin of the coordinate system one unit cell distance to the right along the y axis; thus, this is a $(\bar{1}10)$ plane, as summarized below.

	\bar{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		$(\bar{1}10)$	

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)	

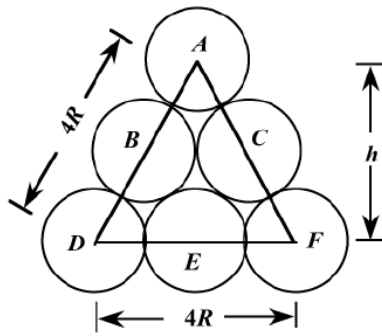
3.75 (a) In the figure below is shown a (100) plane for an FCC unit cell.



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

$$\begin{aligned}
 PD_{100} &= \frac{\text{number of atoms centered on } (100) \text{ plane}}{\text{area of } (100) \text{ plane}} \\
 &= \frac{2 \text{ atoms}}{8R^2} = \frac{1}{4R^2}
 \end{aligned}$$

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

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

And, thus, the planar density is

$$\begin{aligned} \text{PD}_{111} &= \frac{\text{number of atoms centered on (111) plane}}{\text{area of (111) plane}} \\ &= \frac{2 \text{ atoms}}{4R^2\sqrt{3}} = \frac{1}{2R^2\sqrt{3}} \end{aligned}$$

(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

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

3.83 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 3.16 as

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

3.92 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.