SOLUTIONS TO PROBLEMS

PREFACE

This section of instructor's resource materials contains solutions and answers to all problems and questions that appear in the textbook. My penmanship leaves something to be desired; therefore, I generated these solutions/answers using computer software so that the resulting product would be "readable." Furthermore, I endeavored to provide complete and detailed solutions in order that: (1) the instructor, without having to take time to solve a problem, will understand what principles/skills are to be learned by its solution; and (2) to facilitate student understanding/learning when the solution is posted.

I would recommend that the course instructor consult these solutions/answers before assigning problems and questions. In doing so, he or she ensures that the students will be drilled in the intended principles and concepts. In addition, the instructor may provide appropriate hints for some of the more difficult problems.

With regard to symbols, in the text material I elected to boldface those symbols that are italicized in the textbook. Furthermore, I also endeavored to be consistent relative to symbol style. However, in several instances, symbols that appear in the textbook were not available, and it was necessary to make appropriate substitutions. These include the following: the letter **a** (unit cell edge length, crack length) is used in place of the cursive **a**. And Roman **E** and **F** replace script **E** (electric field in Chapter 18) and script **F** (Faraday's constant in Chapter 17), respectively.

I have exercised extreme care in designing these problems/questions, and then in solving them. However, no matter how careful one is with the preparation of a work such as this, errors will always remain in the final product. Therefore, corrections, suggestions, and comments from instructors who use the textbook (as well as their teaching assistants) pertaining to homework problems/solutions are welcomed. These may be sent to me in care of the publisher.

CHAPTER 2

ATOMIC STRUCTURE AND INTERATOMIC BONDING

PROBLEM SOLUTIONS

2.1 (a) When two or more atoms of an element have different atomic masses, each is termed an **isotope**.

(b) The atomic weights of the elements ordinarily are not integers because: (1) the atomic masses of the atoms generally are not integers (except for ^{12}C), and (2) the atomic weight is taken as the weighted average of the atomic masses of an atom's naturally occurring isotopes.

2.2 Atomic mass is the mass of an individual atom, whereas atomic weight is the average (weighted) of the atomic masses of an atom's naturally occurring isotopes.

2.3 (a) In order to determine the number of grams in one amu of material, appropriate manipulation of the amu/atom, g/mol, and atom/mol relationships is all that is necessary, as

$$\#\ \text{g/amu} = \left(\frac{1\ \text{mol}}{6.023\ \text{x}\ 10^{23}\ \text{atoms}}\right)\left(\frac{1\ \text{g/mol}}{1\ \text{amu/atom}}\right)$$

$$= 1.66 \times 10^{-24}\ \text{g/amu}$$

(b) Since there are 453.6 g/lb_m,

$$1\ \text{lb-mol} = \left(453.6\ \text{g/lb}_m\right)\left(6.023 \times 10^{23}\ \text{atoms/g-mol}\right)$$

$$= 2.73 \times 10^{26}\ \text{atoms/lb-mol}$$

2.4 (a) Two important quantum-mechanical concepts associated with the Bohr model of the atom are that electrons are particles moving in discrete orbitals, and electron energy is quantized into shells.

(b) Two important refinements resulting from the wave-mechanical atomic model are that electron position is described in terms of a probability distribution, and electron energy is quantized into both shells and subshells--each electron is characterized by four quantum numbers.

2.5 The **n** quantum number designates the electron shell.

The **l** quantum number designates the electron subshell.
The $\mathbf{m_l}$ quantum number designates the number of electron states in each electron subshell.
The $\mathbf{m_s}$ quantum number designates the spin moment on each electron.

2.6 For the **L** state, **n** = 2, and eight electron states are possible. Possible **l** values are 0 and 1, while possible $\mathbf{m_l}$ values are 0 and ±1. Therefore, for the **s** states, the quantum numbers are $200(\frac{1}{2})$ and $200(-\frac{1}{2})$. For the **p** states, the quantum numbers are $210(\frac{1}{2})$, $210(-\frac{1}{2})$, $211(\frac{1}{2})$, $211(-\frac{1}{2})$, $21(-1)(\frac{1}{2})$, and $21(-1)(-\frac{1}{2})$.

For the **M** state, **n** = 3, and 18 states are possible. Possible **l** values are 0, 1, and 2; possible $\mathbf{m_l}$ values are 0, ±1, and ±2; and possible $\mathbf{m_s}$ values are $\pm\frac{1}{2}$. Therefore, for the **s** states, the quantum numbers are $300(\frac{1}{2})$, $300(-\frac{1}{2})$, for the **p** states they are $310(\frac{1}{2})$, $310(-\frac{1}{2})$, $311(\frac{1}{2})$, $311(-\frac{1}{2})$, $31(-1)(\frac{1}{2})$, and $31(-1)(-\frac{1}{2})$; for the **d** states they are $320(\frac{1}{2})$, $320(-\frac{1}{2})$, $321(\frac{1}{2})$, $321(-\frac{1}{2})$, $32(-1)(\frac{1}{2})$, $32(-1)(-\frac{1}{2})$, $322(\frac{1}{2})$, $322(-\frac{1}{2})$, $32(-2)(\frac{1}{2})$, and $32(-2)(-\frac{1}{2})$.

2.7 The electron configurations of the ions are determined using Table 2.2.

Fe^{2+} - $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6$
Fe^{3+} - $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5$
Cu^{+} - $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10}$
Ba^{2+} - $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^6$
Br^{-} - $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$
S^{2-} - $1s^2 2s^2 2p^6 3s^2 3p^6$

2.8 The Na^{+} ion is just a sodium atom that has lost one electron; therefore, it has an electron configuration the same as neon (Figure 2.6).

The Cl^{-} ion is a chlorine atom that has acquired one extra electron; therefore, it has an electron configuration the same as argon.

2.9 Each of the elements in Group IIA has two **s** electrons.

2.10 (a) The $1s^2 2s^2 2p^6 3s^2 3p^6 3d^7 4s^2$ electron configuration is that of a transition metal because of an incomplete **d** subshell.

(b) The $1s^2 2s^2 2p^6 3s^2 3p^6$ electron configuration is that of an inert gas because of filled 3**s** and 3**p** subshells.

(c) The $1s^2 2s^2 2p^5$ electron configuration is that of a halogen because it is one electron deficient from having a filled **L** shell.

(d) The $1s^2 2s^2 2p^6 3s^2$ electron configuration is that of an alkaline earth metal because of two **s** electrons.

(e) The $1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 4s^2$ electron configuration is that of a transition metal because of an incomplete **d** subshell.

(f) The $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$ electron configuration is that of an alkali metal because of a single **s** electron.

2.11 (a) The 4**f** subshell is being filled for the rare earth series of elements.

(b) The 5**f** subshell is being filled for the actinide series of elements.

2.12 The attractive force between two ions $\mathbf{F_A}$ is just the derivative with respect to the interatomic separation of the attractive energy expression, Equation (2.8), which is just

$$F_A = \frac{dE_A}{dr} = \frac{d\left(-\frac{A}{r}\right)}{dr} = \frac{A}{r^2}$$

The constant **A** in this expression is defined in footnote 3. Since the valences of the Ca^{2+} and O^{2-} ions ($\mathbf{Z_1}$ and $\mathbf{Z_2}$) are both 2, then

$$F_A = \frac{(Z_1 e)(Z_2 e)}{4\pi\varepsilon_o r^2}$$

$$= \frac{(2)(2)\left(1.6 \times 10^{-19}\ C\right)^2}{(4)(\pi)\left(8.85 \times 10^{-12}\ F/m\right)\left(1.25 \times 10^{-9}\ m\right)^2}$$

$$= 5.89 \times 10^{-10}\ N$$

2.13 (a) Differentiation of Equation (2.11) yields

$$\frac{dE_N}{dr} = \frac{A}{r^{(1+1)}} - \frac{nB}{r^{(n+1)}} = 0$$

(b) Now, solving for **r** (= $\mathbf{r_o}$)

$$\frac{A}{r_o^2} = \frac{nB}{r_o^{(n+1)}}$$

or

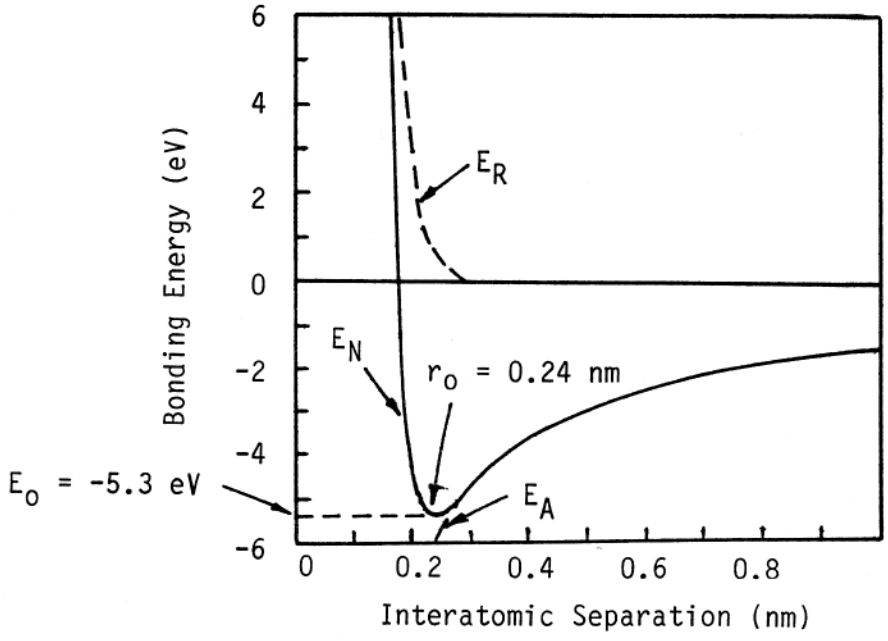
$$r_o = \left(\frac{A}{nB}\right)^{1/(1-n)}$$

(c) Substitution for $\mathbf{r_o}$ into Equation (2.11) and solving for **E** (= $\mathbf{E_o}$)

$$E_o = -\frac{A}{r_o} + \frac{B}{r_o^n}$$

$$= -\frac{A}{\left(\frac{A}{nB}\right)^{1/(1-n)}} + \frac{B}{\left(\frac{A}{nB}\right)^{n/(1-n)}}$$

2.14 (a) Curves of $\mathbf{E_A}$, $\mathbf{E_R}$, and $\mathbf{E_N}$ are shown on the plot below.



(b) From this plot

$$r_o = 0.24 \text{ nm}$$
$$E_o = -5.3 \text{ eV}$$

(c) From Equation (2.11) for $\mathbf{E_N}$

$$A = 1.436$$
$$B = 7.32 \times 10^{-6}$$
$$n = 8$$

Thus,

$$r_o = \left(\frac{A}{nB}\right)^{1/(1-n)}$$

$$= \left[\frac{1.436}{(8)\left(7.32 \times 10^{-6}\right)}\right]^{1/(1-8)} = 0.236 \text{ nm}$$

and

$$E_o = -\frac{1.436}{\left[\frac{1.436}{(8)\left(7.32 \times 10^{-6}\right)}\right]^{1/(1-8)}} + \frac{7.32 \times 10^{-6}}{\left[\frac{1.436}{(8)\left(7.32 \times 10^{-6}\right)}\right]^{8/(1-8)}}$$

$$= -5.32 \text{ eV}$$

2.15 This problem gives us, for a hypothetical X^+-Y^- ion pair, values for $\mathbf{r_o}$ (0.35 nm), $\mathbf{E_o}$ (-6.13 eV), and **n** (10), and asks that we determine explicit expressions for attractive and repulsive energies of Equations 2.8 and 2.9. In essence, it is necessary to compute the values of **A** and **B** in these equations. Expressions for $\mathbf{r_o}$ and $\mathbf{E_o}$ in terms of **n**, **A**, and **B** were determined in Problem 2.13, which are as follows:

$$r_o = \left(\frac{A}{nB}\right)^{1/(1-n)}$$

$$E_o = -\frac{A}{\left(\frac{A}{nB}\right)^{1/(1 - n)}} + \frac{B}{\left(\frac{A}{nB}\right)^{n/(1 - n)}}$$

Thus, we have two simultaneous equations with two unknowns (viz. **A** and **B**). Upon substitution of values for $\mathbf{r_o}$ and $\mathbf{E_o}$ in terms of **n**, these equations take the forms

$$0.35\ \text{nm} = \left(\frac{A}{10B}\right)^{1/(1 - 10)}$$

$$-6.13\ \text{eV} = -\frac{A}{\left(\frac{A}{10B}\right)^{1/(1 - 10)}} + \frac{B}{\left(\frac{A}{10B}\right)^{10/(1 - 10)}}$$

Simultaneous solution of these two equations leads to **A** = 2.38 and **B** = 1.88 x 10^{-5}. Thus, Equations (2.8) and (2.9) become

$$E_A = -\frac{2.38}{r}$$

$$E_R = \frac{1.88 \times 10^{-5}}{r^{10}}$$

Of course these expressions are valid for **r** and **E** in units of nanometers and electron volts, respectively.

2.16 (a) Differentiating Equation (2.12) with respect to **r** yields

$$\frac{dE}{dr} = \frac{C}{r^2} - \frac{De^{-r/\rho}}{\rho}$$

At $\mathbf{r} = \mathbf{r_o}$, d**E**/d**r** = 0, and

$$\frac{C}{r_o^{\,2}} = \frac{De^{-(r_o/\rho)}}{\rho} \qquad (2.12b)$$

Solving for **C** and substitution into Equation (2.12) yields an expression for $\mathbf{E_o}$ as

$$E_o = De^{-(r_o/\rho)}\left(1 - \frac{r_o}{\rho}\right)$$

(b) Now solving for **D** from Equation (2.12b) above yields

$$D = \frac{C\rho e^{(r_o/\rho)}}{r_o^2}$$

Substitution of this expression for **D** into Equation (2.12) yields an expression for $\mathbf{E_o}$ as

$$E_o = \frac{C}{r_o}\left(\frac{\rho}{r_o} - 1\right)$$

2.17 (a) The main differences between the various forms of primary bonding are:

Ionic--there is electrostatic attraction between oppositely charged ions.

Covalent--there is electron sharing between two adjacent atoms such that each atom assumes a stable electron configuration.

Metallic--the positively charged ion cores are shielded from one another, and also "glued" together by the sea of valence electrons.

(b) The Pauli exclusion principle states that each electron state can hold no more than two electrons, which must have opposite spins.

2.18 Covalently bonded materials are less dense than metallic or ionically bonded ones because covalent bonds are directional in nature whereas metallic and ionic are not; when bonds are directional, the atoms cannot pack together in as dense a manner, yielding a lower mass density.

2.19 The percent ionic character is a function of the electron negativities of the ions $\mathbf{X_A}$ and $\mathbf{X_B}$ according to Equation (2.10). The electronegativities of the elements are found in Figure 2.7.

For MgO, $\mathbf{X_{Mg}}$ = 1.2 and $\mathbf{X_O}$ = 3.5, and therefore,

$$\%IC = \left[1 - \mathbf{e}^{(-0.25)(3.5-1.2)^2}\right] \times 100 = 73.4\%$$

For GaP, $\mathbf{X_{Ga}}$ = 1.6 and $\mathbf{X_P}$ = 2.1, and therefore,

$$\%IC = \left[1 - e^{(-0.25)(2.1-1.6)^2}\right] \times 100 = 6.1\%$$

For CsF, X_{Cs} = 0.7 and X_F = 4.0, and therefore,

$$\%IC = \left[1 - e^{(-0.25)(4.0-0.7)^2}\right] \times 100 = 93.4\%$$

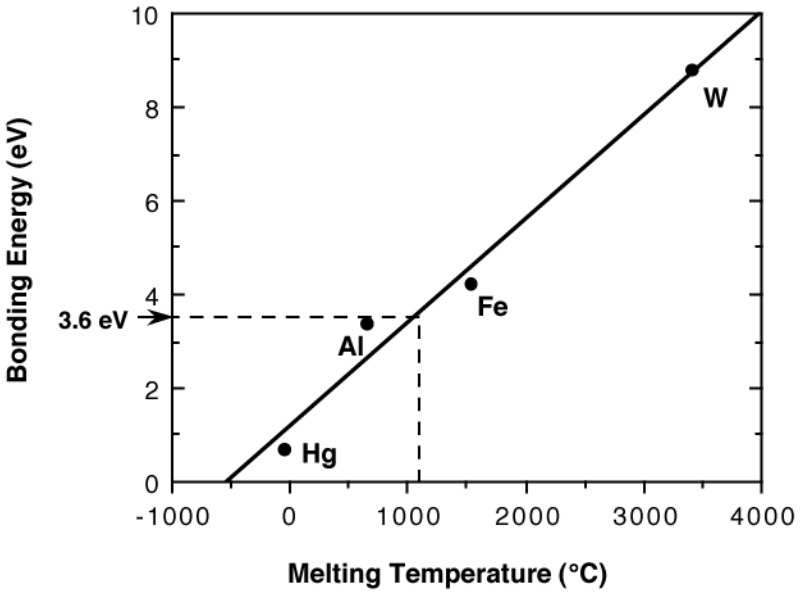
For CdS, X_{Cd} = 1.7 and X_S = 2.5, and therefore,

$$\%IC = \left[1 - e^{(-0.25)(2.5-1.7)^2}\right] \times 100 = 14.8\%$$

For FeO, X_{Fe} = 1.8 and X_O = 3.5, and therefore,

$$\%IC = \left[1 - e^{(-0.25)(3.5-1.8)^2}\right] \times 100 = 51.4\%$$

2.20 Below is plotted the bonding energy versus melting temperature for these four metals. From this plot, the bonding energy for copper (melting temperature of 1084°C) should be approximately 3.6 eV. The experimental value is 3.5 eV.



2.21 For silicon, having the valence electron structure $3s^2 3p^2$, **N'** = 4; thus, there are 8 - **N'** = 4 covalent bonds per atom.

For bromine, having the valence electron structure $4s^2 4p^5$, **N'** = 7; thus, there is 8 - **N'** = 1 covalent bond per atom.

For nitrogen, having the valence electron structure $2s^2 2p^3$, **N'** = 5; thus, there are 8 - **N'** = 3 covalent bonds per atom.

For sulfur, having the valence electron structure $3s^2 3p^4$, **N'** = 6; thus, there are 8 - **N'** = 2 covalent bonds per atom.

2.22 For brass, the bonding is metallic since it is a metal alloy.

For rubber, the bonding is covalent with some van der Waals. (Rubber is composed primarily of carbon and hydrogen atoms.)

For BaS, the bonding is predominantly ionic (but with some covalent character) on the basis of the relative positions of Ba and S in the periodic table.

For solid xenon, the bonding is van der Waals since xenon is an inert gas.

For bronze, the bonding is metallic since it is a metal alloy (composed of copper and tin).

For nylon, the bonding is covalent with perhaps some van der Waals. (Nylon is composed primarily of carbon and hydrogen.)

For AlP the bonding is predominantly covalent (but with some ionic character) on the basis of the relative positions of Al and P in the periodic table.

2.23 The intermolecular bonding for HF is hydrogen, whereas for HCl, the intermolecular bonding is van der Waals. Since the hydrogen bond is stronger than van der Waals, HF will have a higher melting temperature.

2.24 The geometry of the H_2O molecules, which are hydrogen bonded to one another, is more restricted in the solid phase than for the liquid. This results in a more open molecular structure in the solid, and a less dense solid phase.

CHAPTER 3

THE STRUCTURE OF CRYSTALLINE SOLIDS

PROBLEM SOLUTIONS

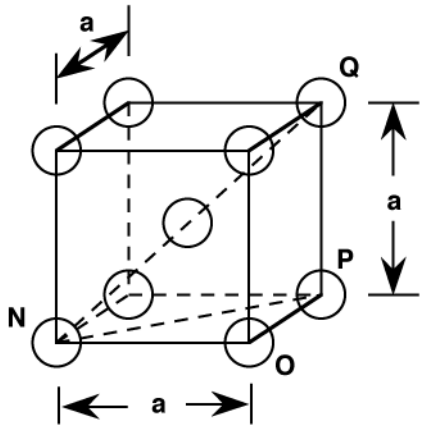
3.1 Atomic structure relates to the number of protons and neutrons in the nucleus of an atom, as well as the number and probability distributions of the constituent electrons. On the other hand, crystal structure pertains to the arrangement of atoms in the crystalline solid material.

3.2 A crystal structure is described by both the geometry of, and atomic arrangements within, the unit cell, whereas a crystal system is described only in terms of the unit cell geometry. For example, face-centered cubic and body-centered cubic are crystal structures that belong to the cubic crystal system.

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

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

3.4 This problem calls for a demonstration of the relationship $\mathbf{a} = 4\mathbf{R}\sqrt{3}$ 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**,

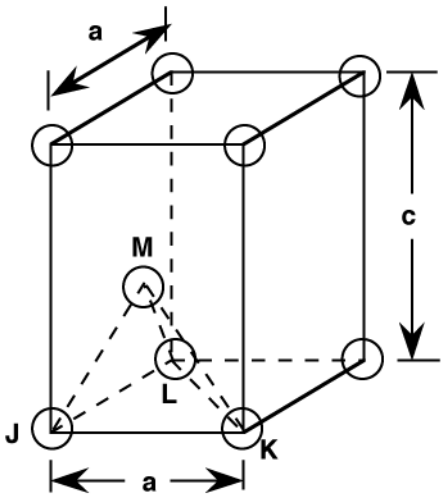
$$(\overline{NQ})^2 = (\overline{QP})^2 + (\overline{NP})^2$$

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

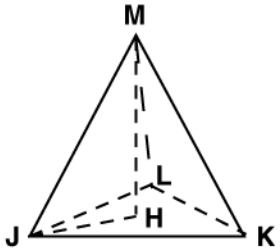
$$(4R)^2 = a^2 + 2a^2, \text{ or}$$

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

3.5 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 $\overline{\mathbf{MH}} = \mathbf{c}/2$. And, since atoms at points **J**, **K**, and **M**, all touch one another,

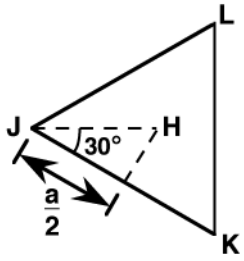
$$\overline{JM} = \overline{JK} = 2R = a$$

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

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

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

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



$$\cos 30^\circ = \frac{a/2}{JH} = \frac{\sqrt{3}}{2}, \text{ and}$$

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

Substituting this value for $\overline{\mathbf{JH}}$ 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**

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

3.6 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

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

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 $\mathbf{V_C = a^3}$. But **a** depends on **R** according to Equation (3.3), and

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

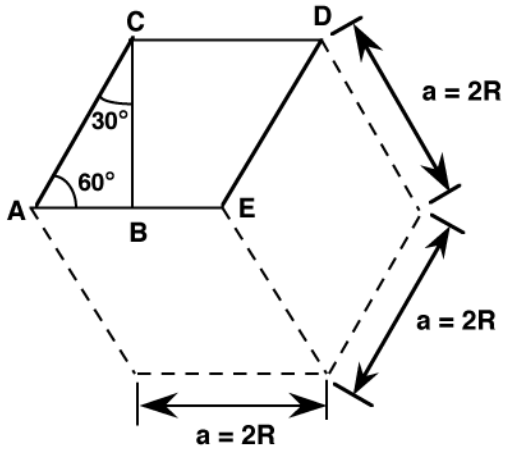
Thus,

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

3.7 This problem calls for a demonstration that the **APF** for HCP is 0.74. Again, the **APF** is just the total sphere-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 $\overline{\mathbf{CD}}$ times the height $\overline{\mathbf{BC}}$. But $\overline{\mathbf{CD}}$ 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** = 1.633**a** = 2**R**(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,

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

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

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

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

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

Thus,

$$\rho = \frac{(2 \text{ atoms/unit cell})(55.9 \text{ g/mol})}{\left\{\left[(4)\left(0.124 \times 10^{-7} \text{ cm}\right)^3/\sqrt{3}\right]^3/(\text{unit cell})\right\}\left(6.023 \times 10^{23} \text{ atoms/mol}\right)}$$

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

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

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

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

And solving for **R** from the above two expressions yields

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

$$= \left[\frac{(4 \text{ atoms/unit cell})(192.2 \text{ g/mol})}{(\sqrt{2})(16)\left(22.4 \text{ g/cm}^3\right)\left(6.023 \times 10^{23} \text{ atoms/mol}\right)}\right]^{1/3}$$

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

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

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

Since,

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

and solving for **R**

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

$$= \left[\frac{\left(3\sqrt{3}\right)(2 \text{ atoms/unit cell})(50.9 \text{ g/mol})}{(64)\left(5.96 \text{ g/cm}^3\right)\left(6.023 \times 10^{23} \text{ atoms/mol}\right)} \right]^{1/3}$$

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

3.11 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** = 2**R**. Therefore, employment of Equation (3.5) yields

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

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

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

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

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

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

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

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

(b) From the solution to Problem 3.7, since **a** = 2**R**, then, for HCP

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

but, since **c** = 1.58**a**

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

Now, solving for **a**

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

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

And finally

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

3.13 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 $\mathbf{V_C} = \left(2R\sqrt{2}\right)^3$. Also, **R** = 0.143 nm (1.43 x 10^{-8} cm) and $\mathbf{A_{Al}}$ = 26.98 g/mol. Employment of Equation (3.5) yields

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

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

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

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

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

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

Magnesium has an HCP crystal structure, and from Problem 3.7,

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

and, since **c** = 1.624**a** and **a** = 2**R** = 2(1.60 x 10^{-8} cm) = 3.20 x 10^{-8} cm

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

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

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

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

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

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

Tungsten has a BCC crystal structure for which **n** = 2 and **a** = $\frac{4\mathbf{R}}{\sqrt{3}}$; also $\mathbf{A_W}$ = 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.

3.14 In order to determine whether Nb has an FCC or BCC crystal structure, we need to compute its density for each of the crystal structures. For FCC, **n** = 4, and **a** = $2\mathbf{R}\sqrt{2}$. Also, from Figure 2.6, its atomic weight is 92.91 g/mol. Thus, for FCC

$$\rho = \frac{nA_{Nb}}{\left(2R\sqrt{2}\right)^3 N_A}$$

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

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

For BCC, **n** = 2, and **a** = $\frac{4\mathbf{R}}{\sqrt{3}}$, thus

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

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

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

3.15 For each of these three alloys we need to, by trial and error, 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 $4R/\sqrt{3}$.

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

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

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

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

Therefore, its crystal structure is BCC.

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

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

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

Therefore, its crystal structure is simple cubic.

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

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

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

Therefore, its crystal structure is BCC.

3.16 In order to determine the **APF** for U, we need to compute both the unit cell volume ($\mathbf{V_C}$) which is just the product of the three unit cell parameters, as well as the total sphere volume ($\mathbf{V_S}$) which is just the product of the volume of a single sphere and the number of spheres in the unit cell (**n**). The value of **n** may be calculated from Equation (3.5) as

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

$$= \frac{(19.05)(2.86)(5.87)(4.95)\left(\times 10^{-24}\right)\left(6.023 \times 10^{23}\right)}{283.03}$$

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

Therefore

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

$$= \frac{(4)\left[\frac{4}{3}(\pi)(0.1385)^3\right]}{(0.286)(0.587)(0.495)}$$

$$= 0.536$$

3.17 (a) From the definition of the **APF**

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

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

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

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

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

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

$$\rho = \frac{nA_{In}}{a^2 c N_A}$$

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

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

3. 18 (a) We are asked to calculate the unit cell volume for Be. From the solution to Problem 3.7

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

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

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

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

(b) The density of Be is determined as follows:

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

For HCP, **n** = 6 atoms/unit cell, and for Be, $\mathbf{A_{Be}}$ = 9.01 g/mol. 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.

3.19 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 3.7 it was shown that

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

In this case **c** = 1.624(2**R**). Making this substitution into the previous equation, and then solving for **R** using Equation (3.5) yields

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

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

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

3.20 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 3.7, that is

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

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

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

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

3.21 (a) The unit cell shown in the problem 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

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

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

Thus,

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

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

$$= 8.50 \text{ g/cm}^3$$

3.22 First of all, open 'Notepad" in Windows. Now enter into "Notepad" commands to generate the $AuCu_3$ unit cell. One set of commands that may be used is as follows:

```
[DisplayProps]
Rotatez=-30
Rotatey=-15

[AtomProps]
Gold=LtRed,0.14
Copper=LtYellow,0.13

[BondProps]
SingleSolid=LtGray

[Atoms]
Au1=1,0,0,Gold
Au2=0,0,0,Gold
Au3=0,1,0,Gold
Au4=1,1,0,Gold
Au5=1,0,1,Gold
Au6=0,0,1,Gold
```

```
Au7=0,1,1,Gold
Au8=1,1,1,Gold
Cu1=0.5,0,0.5,Copper
Cu2=0,0.5,0.5,Copper
Cu3=0.5,1,0.5,Copper
Cu4=1,0.5,0.5,Copper
Cu5=0.5,0.5,1,Copper
Cu6=0.5,0.5,0,Copper

[Bonds]
B1=Au1,Au5,SingleSolid
B2=Au5,Au6,SingleSolid
B3=Au6,Au2,SingleSolid
B4=Au2,Au1,SingleSolid
B5=Au4,Au8,SingleSolid
B6=Au8,Au7,SingleSolid
B7=Au7,Au3,SingleSolid
B8=Au3,Au4,SingleSolid
B9=Au1,Au4,SingleSolid
B10=Au8,Au5,SingleSolid
B11=Au2,Au3,SingleSolid
B12=Au6,Au7,SingleSolid
```

Under the "File" menu of "Note Pad," click "Save As", and then assign the file for this figure a name followed by a period and "mdf"; for example, “AuCu3.mdf”. And, finally save this file in the “mdf” file inside of the “Interactive MSE” folder (which may be found in its installed location).

Now, in order to view the unit cell just generated, bring up “Interactive MSE”, and then open any one of the three submodules under “Crystallinity and Unit Cells” or the “Ceramic Structures” module. Next select “Open” under the “File” menu, and then open the “mdf” folder. Finally, select the name you assigned to the item in the window that appears, and hit the “OK” button. The image that you generated will now be displayed.

3.23 First of all, open ‘Notepad” in Windows.. Now enter into “Notepad” commands to generate the AuCu unit cell. One set of commands that may be used is as follows:

```
[DisplayProps]
Rotatez=-30
Rotatey=-15

[AtomProps]
Gold=LtRed,0.14
Copper=LtYellow,0.13

[BondProps]
SingleSolid=LtGray

[Atoms]
Au1=0,0,0,Gold
Au2=1,0,0,Gold
Au3=1,1,0,Gold
Au4=0,1,0,Gold
Au5=0,0,1.27,Gold
Au6=1,0,1.27,Gold
```

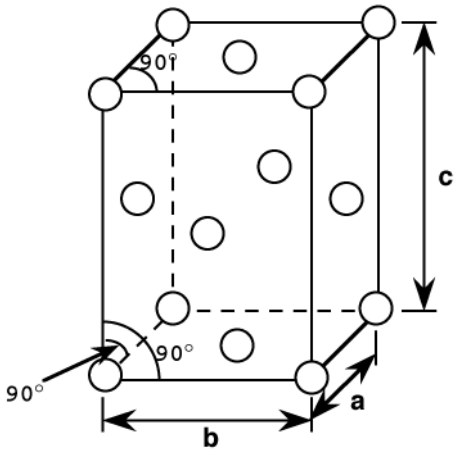
Au7=1,1,1.27,Gold
Au8=0,1,1.27,Gold
Cu1=0.5,0.5,0.635,Copper

[Bonds]
B1=Au1,Au2,SingleSolid
B2=Au2,Au3,SingleSolid
B3=Au3,Au4,SingleSolid
B4=Au1,Au4,SingleSolid
B5=Au5,Au6,SingleSolid
B6=Au6,Au7,SingleSolid
B7=Au7,Au8,SingleSolid
B8=Au5,Au8,SingleSolid
B9=Au1,Au5,SingleSolid
B10=Au2,Au6,SingleSolid
B11=Au3,Au7,SingleSolid
B12=Au4,Au8,SingleSolid

Under the "File" menu of "Note Pad," click "Save As", and then assign the file for this figure a name followed by a period and "mdf"; for example, “AuCu.mdf”. And, finally save this file in the “mdf” file inside of the “Interactive MSE” folder (which may be found in its installed location).

Now, in order to view the unit cell just generated, bring up “Interactive MSE”, and then open any one of the three submodules under “Crystallinity and Unit Cells” or the “Ceramic Structures” module. Next select “Open” under the “File” menu, and then open the “mdf” folder. Finally, select the name you assigned to the item in the window that appears, and hit the “OK” button. The image that you generated will now be displayed.

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



3.25 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 only 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 $\frac{1}{2}1\frac{1}{2}$.

3.26 (a) 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 $\frac{1}{2}1\frac{1}{2}$.

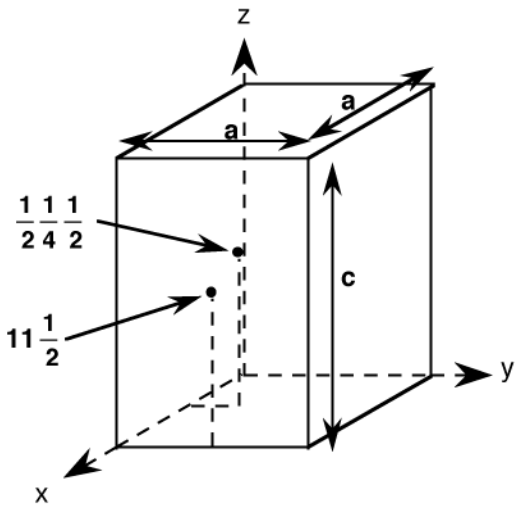
Furthermore, the sodium ions are situated at the centers of all unit cell edges, and, in addition, at the unit cell center. For the bottom face of the unit cell, the point coordinates are as follows: $\frac{1}{2}00$, $1\frac{1}{2}0$, $\frac{1}{2}10$, $0\frac{1}{2}0$. While, for the horizontal plane that passes through the center of the unit cell (which includes the ion at the unit cell center), the coordinates are $00\frac{1}{2}$, $10\frac{1}{2}$, $\frac{1}{2}\frac{1}{2}\frac{1}{2}$, $11\frac{1}{2}$, and $01\frac{1}{2}$. And for the four ions on the top face $\frac{1}{2}01$, $1\frac{1}{2}1$, $\frac{1}{2}11$, and $0\frac{1}{2}1$.

(b) This portion of the 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.

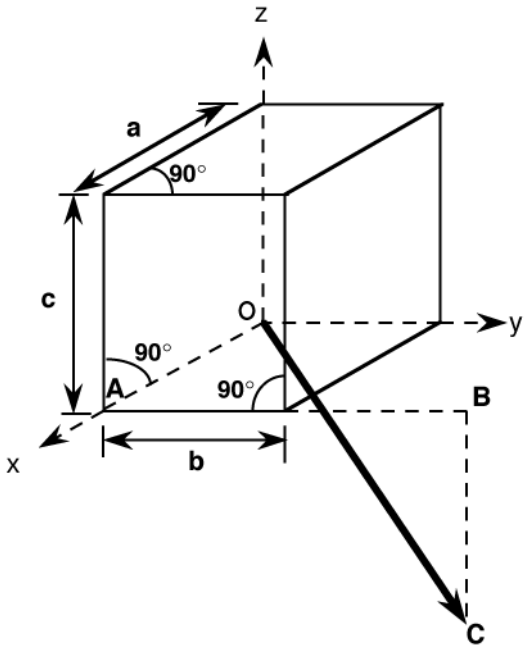
First of all, the sulfur atoms occupy the face-centered positions in the unit cell, which from the solution to Problem 3.25, are as follows: 000, 100, 110, 010, 001, 101, 111, 011, $\frac{1}{2}\frac{1}{2}0$, $\frac{1}{2}\frac{1}{2}1$, $1\frac{1}{2}\frac{1}{2}$, $0\frac{1}{2}\frac{1}{2}$, $\frac{1}{2}0\frac{1}{2}$, 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 $\frac{3}{4}\frac{3}{4}\frac{3}{4}$.

3.27 A tetragonal unit in which are shown the $11\frac{1}{2}$ and $\frac{1}{2}\frac{1}{4}\frac{1}{2}$ point coordinates is presented below.

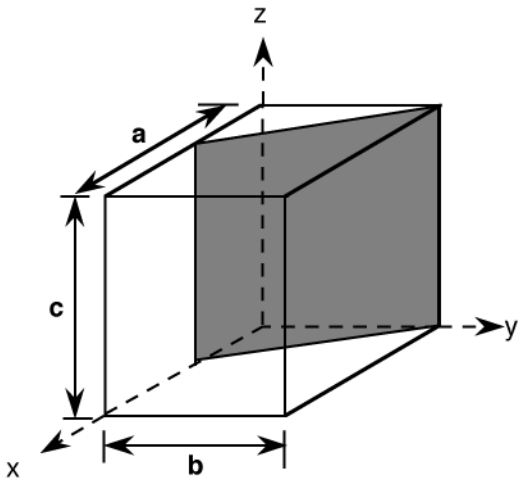


3.28 This portion of the problem calls for us to draw a $[12\bar{1}]$ direction within an orthorhombic unit cell (**a** ≠ **b** ≠ **c**, $\alpha = \beta = \gamma = 90°$). Such a unit cell with its origin positioned at point **O** is shown below. We first move along the +**x**-axis **a** units (from point **O** to point **A**), then parallel to the +**y**-axis 2**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 $[12\bar{1}]$ direction is the vector from the origin (point **O**) to point **C** as shown.

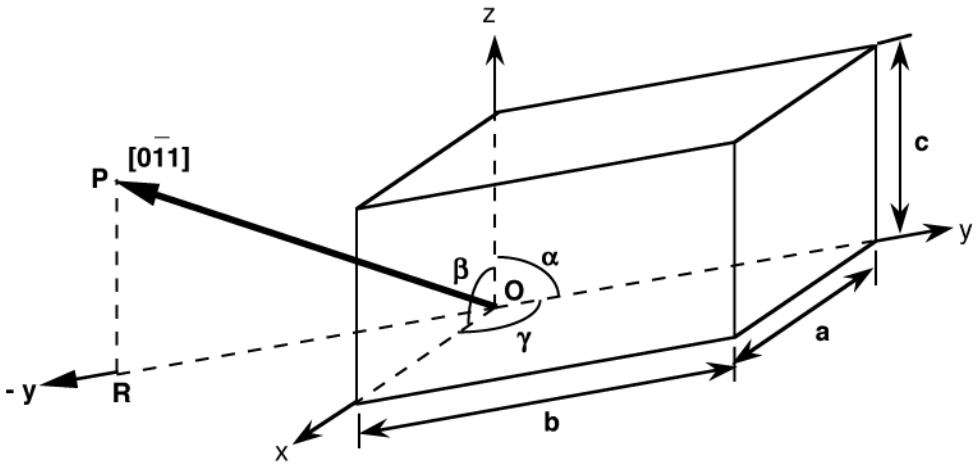


We are now asked to draw a (210) plane within an orthorhombic unit cell. First remove the three indices from the parentheses, and take their reciprocals--i.e., 1/2, 1, and ∞. This means that the

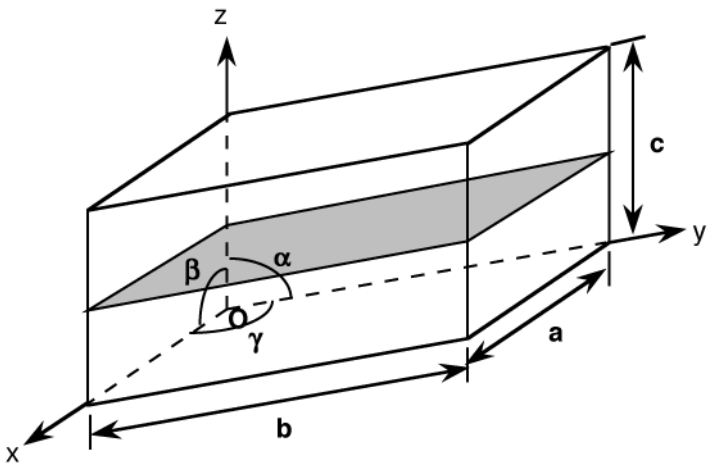
plane intercepts the **x**-axis at **a**/2, the **y**-axis at **b**, and parallels the **z**-axis. The plane that satisfies these requirements has been drawn within the orthorhombic unit cell below.



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



(b) A (002) plane is drawn within the monoclinic cell shown below. We first remove the parentheses and take the reciprocals of the indices; this gives ∞, ∞, and 1/2. Thus, the (002) plane parallels both **x**- and **y**-axes, and intercepts the **z**-axis at **c**/2, as indicated in the drawing.



3.30 (a) We are asked for the indices of the two directions sketched in the figure. For direction **1**, the projection on the **x**-axis is zero (since it lies in the **y**-**z** plane), while projections on the **y**- and **z**-axes are **b**/2 and **c**, respectively. This is an [012] direction as indicated in the summary below

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

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

	x	y	z
Projections	a/2	b/2	- c
Projections in terms of **a**, **b**, and **c**	1/2	1/2	-1
Reduction to integers	1	1	-2

Enclosure $[11\bar{2}]$

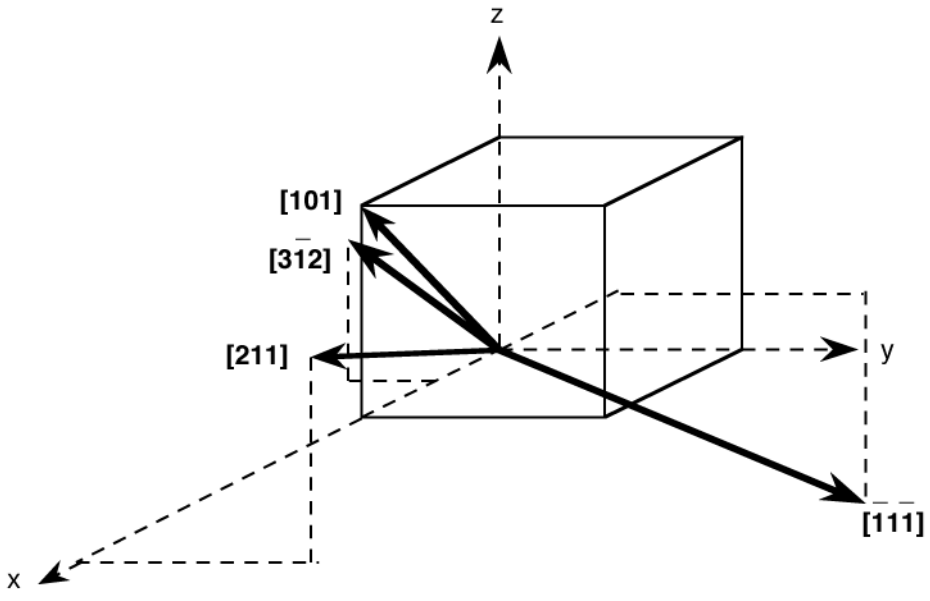
(b) This part of the problem calls for the indices of the two planes which are drawn in the sketch. Plane **1** is an (020) plane. The determination of its indices is summarized below.

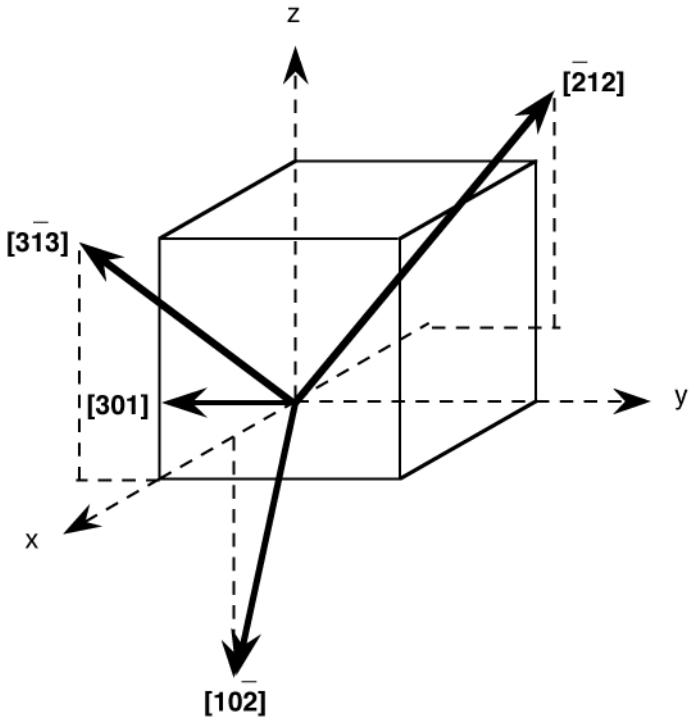
	x	y	z
Intercepts	∞ a	b/2	∞ c
Intercepts in terms of **a**, **b**, and **c**	∞	1/2	∞
Reciprocals of intercepts	0	2	0
Enclosure		(020)	

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

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

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





3.32 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		$[1\bar{2}1]$	

3.33 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		$[\bar{1}1\bar{1}]$	

3.34 For tetragonal crystals **a** = **b** ≠ **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 $[0\bar{1}0]$.

3.35 (a) We are asked to convert [100] and [111] directions into the four- index Miller-Bravais scheme for hexagonal unit cells. For [100]

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

From Equations (3.6)

$$u = \frac{n}{3}(2u' - v') = \frac{n}{3}(2 - 0) = \frac{2n}{3}$$

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

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

$$w = nw' = 0$$

If we let **n** = 3, then **u** = 2, **v** = -1, **t** = -1, and **w** = 0. Thus, the direction is represented as [**uvtw**] = $[2\bar{1}\bar{1}0]$.

For [111], **u'** = 1, **v'** = 1, and **w'** = 1; therefore,

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

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

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

$$w = n$$

If we again let **n** = 3, then **u** = 1, **v** = 1, **t** = -2, and **w** = 3. Thus, the direction is represented as $[11\bar{2}3]$.

(b) This portion of the problem asks for the same conversion of the (010) and (101) planes. A plane for hexagonal is represented by (**hkil**) where **i** = - (**h** + **k**), and **h**, **k**, and **l** are the same for both systems. For the (010) plane, **h** = 0, **k** = 1, **l** = 0, and

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

Thus, the plane is now represented as (**hkil**) = $(01\bar{1}0)$.

For the (101) plane, **i** = - (1 + 0) = -1, and (**hkil**) = $(10\bar{1}1)$.

3.36 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		$(11\bar{1})$	

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)	

3.37 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)	

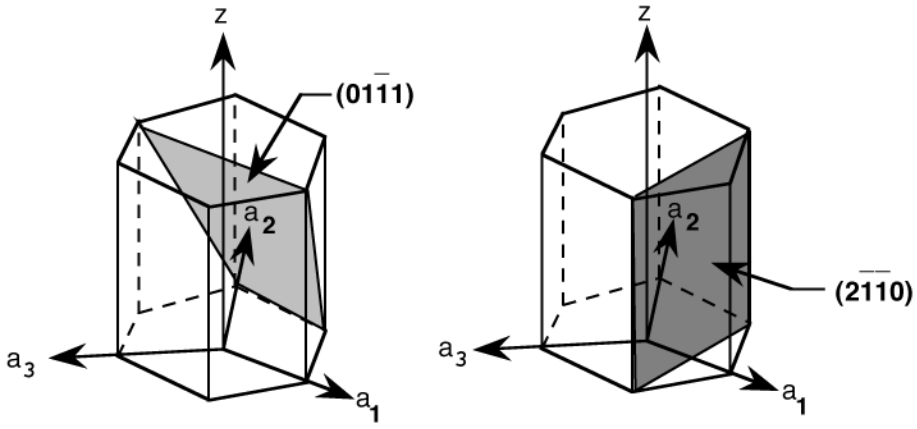
3.38 For plane **A** since the plane passes through the origin of the coordinate system as shown, we will move the origin of the coordinate system one unit cell distance vertically along the **z** axis; thus, this is a $(21\bar{1})$ plane, as summarized below.

	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		$(21\bar{1})$	

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 $(02\bar{1})$ plane, as summarized below.

	x	y	z
Intercepts	∞ 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		$(02\bar{1})$	

3.39 The $(01\bar{1}1)$ and $(2\bar{1}\bar{1}0)$ planes in a hexagonal unit cell are shown below.



3.40 (a) For this plane we will leave the origin of the coordinate system as shown; thus, this is a $(1\bar{2}11)$ plane, as summarized below.

	a_1	a_2	a_3	z
Intercepts	a	$-\frac{a}{2}$	a	c
Intercepts in terms of **a**'s and **c**	1	$-\frac{1}{2}$	1	1
Reciprocals of intercepts	1	- 2	1	1
Reduction		not necessary		
Enclosure		$(1\bar{2}11)$		

(b) For this plane we will leave the origin of the coordinate system as shown; thus, this is a $(2\bar{1}\,\bar{1}2)$ plane, as summarized below.

	a_1	a_2	a_3	z
Intercepts	a/2	-a	-a	c/2
Intercepts in terms of **a**'s and **c**	1/2	-1	-1	1/2
Reciprocals of intercepts	2	-1	-1	2
Reduction		not necessary		
Enclosure		$(2\bar{1}\,\bar{1}2)$		

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