2.1 What is the mass in grams of (a) a proton, (b) a neutron, and (c) an electron?
(a) mass of proton = $1.673 \times 10^{-24}$ g  
(b) mass of neutron = $1.675 \times 10^{-24}$ g  
(c) mass of electron = $9.109 \times 10^{-28}$ g

2.2 What is the electric charge in coulombs of (a) a proton, (b) a neutron, and (c) an electron?
(a) proton charge = $+1.602 \times 10^{-19}$ C  
(b) neutron charge = 0 C  
(c) electron charge = $-1.602 \times 10^{-19}$ C

2.3 Define (a) atomic number, (b) atomic mass unit, (c) Avogadro’s number, and (d) relative gram atomic mass.
(a) The atomic number is the number of protons contained in the nucleus of an atom.
(b) An atomic mass unit, u, is defined as exactly 1/12 of the mass of the carbon atom which has a mass of 12 u.
(c) Avogadro’s number, $N_A$, is $6.02 \times 10^{23}$ atoms/mol.
(d) The relative gram atomic mass of an element is the mass in grams of $6.023 \times 10^{23}$ atoms of that element.

2.4 What is the mass in grams of one atom of gold?
\[ x = \text{mass of 1 Au atom} = \frac{196.97 \text{ g/mol Au}}{6.02 \times 10^{23} \text{ atoms/mol}} \times (1 \text{ atom}) = 3.27 \times 10^{-22} \text{ g Au} \]

2.5 How many atoms are there in 1 g of gold?
\[ x = \frac{6.02 \times 10^{23} \text{ atoms/mol}}{196.97 \text{ g/mol Au}} \times (1 \text{ g Au}) = 3.06 \times 10^{21} \text{ atoms Au} \]

2.6 A gold wire is 0.70 mm in diameter and 8.0 cm in length. How many atoms does it contain? The density of gold is 19.3 g/cm$^3$.

First determine the mass of gold based upon the wire volume and the density of gold.
\[ m = \text{mass of Au} = \rho V \ \text{where} \ \rho = 19.3 \text{ g/cm}^3 \]
and
\[ V = \text{volume of wire} = (\text{area})(\text{length}) \]
\[ = \left( \frac{\pi d^2}{4} \right)(L) = \frac{\pi}{4} \left[ (0.7 \text{ mm}) \left( \frac{1 \text{ cm}}{10 \text{ mm}} \right) \right]^2 (8.0 \text{ cm}) = 0.0308 \text{ cm}^3 \]

Thus, \( m = (19.3 \text{ g/cm}^3 \text{ Au})(0.0308 \text{ cm}^3) = 0.5944 \text{ g Au} \)

The number of atoms is then calculated as,

\[
\text{No. of atoms Au} = (0.5944 \text{ g Au}) \left[ \frac{6.02 \times 10^{23} \text{ atoms/mol}}{196.97 \text{ g/mol Au}} \right] = 1.82 \times 10^{21} \text{ atoms Au}
\]

2.7 What is the mass in grams of one atom of molybdenum?

\[ x = \text{mass of 1 Mo atom} = \frac{95.94 \text{ g/mol Mo}}{6.02 \times 10^{23} \text{ atoms/mol}} \times (1 \text{ atom}) = 1.59 \times 10^{-22} \text{ g Mo} \]

2.8 How many atoms are there in 1 g of molybdenum?

\[
x = \text{No. of atoms of Mo} = \frac{6.02 \times 10^{23} \text{ atoms/mol}}{95.94 \text{ g/mol Mo}} \times (1 \text{ g Mo}) = 6.27 \times 10^{21} \text{ atoms Mo}
\]

2.9 A solder contains 52 wt % tin and 48 wt % lead. What are the atomic percentages of Sn and Pb in this solder?

Using a basis of 100 g of solder, there are 52 g of Sn and 48 g of Pb. The number of gram-moles of tin and lead is therefore,

\[
\text{No. of gram-moles of Sn} = \frac{52 \text{ g}}{118.69 \text{ g/mol}} = 0.4381 \text{ mol}
\]
\[
\text{No. of gram-moles of Pb} = \frac{48 \text{ g}}{207.19 \text{ g/mol}} = 0.2317 \text{ mol}
\]

Total gram-moles = 0.6698 mol

The atomic percentages may then be calculated as,

\[
\text{Atomic \% Sn} = \left[ \frac{0.4381 \text{ mol}}{0.6698 \text{ mol}} \right] (100\%) = 65.4 \text{ at}\%
\]
\[
\text{Atomic \% Pb} = \left[ \frac{0.2317 \text{ mol}}{0.6698 \text{ mol}} \right] (100\%) = 34.6 \text{ at}\%
\]

2.10 A monel alloy consists of 70 wt % Ni and 30 wt % Cu. What are the atomic percentages of Ni and Cu in this alloy?
Using a basis of 100 g of alloy, there are 70 g of Ni and 30 g of Cu. The number of gram-moles of each element is thus,

\[
\text{No. of gram-moles of Cu} = \frac{30 \text{ g}}{63.54 \text{ g/mol}} = 0.472 \text{ mol}
\]
\[
\text{No. of gram-moles of Ni} = \frac{70 \text{ g}}{58.71 \text{ g/mol}} = 1.192 \text{ mol}
\]
\[
\text{Total gram-moles} = 1.664 \text{ mol}
\]

The atomic percentages may then be calculated as,

\[
\text{Atomic% Cu} = \left[ \frac{0.472 \text{ mol}}{1.664 \text{ mol}} \right] (100\%) = 28.4 \text{ at%}
\]
\[
\text{Atomic% Ni} = \left[ \frac{1.192 \text{ mol}}{1.664 \text{ mol}} \right] (100\%) = 71.6 \text{ at%}
\]

2.11 A cupronickel alloy consists of 80 wt % Cu and 20 wt % Ni. What are the atomic percentages of Cu and Ni in the alloy?

Using a basis of 100 g of alloy, there are 80 g of Cu and 20 g of Ni. The respective number of gram-moles is thus,

\[
\text{No. of gram-moles of Cu} = \frac{80 \text{ g}}{63.54 \text{ g/mol}} = 1.2590 \text{ mol}
\]
\[
\text{No. of gram-moles of Ni} = \frac{20 \text{ g}}{58.71 \text{ g/mol}} = 0.3407 \text{ mol}
\]
\[
\text{Total gram-moles} = 1.5997 \text{ mol}
\]

The atomic percentages may then be calculated as,

\[
\text{Atomic% Cu} = \left[ \frac{1.2590 \text{ mol}}{1.5997 \text{ mol}} \right] (100\%) = 78.7 \text{ at%}
\]
\[
\text{Atomic% Ni} = \left[ \frac{0.3407 \text{ mol}}{1.5997 \text{ mol}} \right] (100\%) = 21.3 \text{ at%}
\]

2.12 What is the chemical formula of an intermetallic compound that consists of 49.18 wt % Cu and 50.82 wt % Au?

We need to determine $\text{Cu}_x\text{Au}_y$, where $x$ and $y$ represent the gram-mole fractions of copper and gold, respectively. Therefore, first calculate the gram-mole fractions of these elements using a basis of 100 g of compound:
No. of gram-moles of Cu = \( \frac{49.18 \text{ g}}{63.54 \text{ g/mol}} = 0.774 \text{ mol} \)

No. of gram-moles of Au = \( \frac{50.82 \text{ g}}{196.97 \text{ g/mol}} = 0.258 \text{ mol} \)

Total gram-moles = \( 1.032 \text{ mol} \)

\[ x = \text{Gram-mole fraction of Cu} = \left( \frac{0.774 \text{ mol}}{1.032 \text{ mol}} \right) = 0.75 \]

\[ y = \text{Gram-mole fraction of Au} = \left( \frac{0.258 \text{ mol}}{1.032 \text{ mol}} \right) = 0.25 \]

Thus we have Cu\(_{0.75}\)Au\(_{0.25}\) or, multiplying by 4, Cu\(_3\)Au.

2.13 What is the chemical formula of an intermetallic compound that consists of 15.68 wt % Mg and 84.32 wt % Al?

The chemical formula, Mg\(_x\)Al\(_y\), may be determined based on the gram-mole fractions of magnesium and aluminum. Using a basis of 100 g of intermetallic compound,

No. of gram-moles of Mg = \( \frac{15.68 \text{ g}}{24.31 \text{ g/mol}} = 0.645 \text{ mol} \)

No. of gram-moles of Al = \( \frac{84.32 \text{ g}}{26.98 \text{ g/mol}} = 3.125 \text{ mol} \)

Total gram-moles = \( 3.770 \text{ mol} \)

\[ x = \text{Gram-mole fraction of Mg} = \left( \frac{0.645 \text{ mol}}{3.770 \text{ mol}} \right) = 0.17 \]

\[ y = \text{Gram-mole fraction of Al} = \left( \frac{3.125 \text{ mol}}{3.770 \text{ mol}} \right) = 0.83 \]

Thus we have Mg\(_{0.17}\)Al\(_{0.83}\) or, multiplying by 6, MgAl\(_5\).

2.14 Define a photon.

A photon is a discrete amount or quantum of energy in the form of electromagnetic radiation.

2.15 Calculate the energy in joules and electron volts of the photon whose wavelength is 303.4 nm.

Using Plank’s equation with \( v = c/\lambda, \)
2.16 Calculate the energy in joules and electron volts of the photon whose wavelength is 226.4 nm.

\[
\Delta E = \frac{hc}{\lambda} = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})(3.00 \times 10^8 \text{ m/s})}{(226.4 \text{ nm})(10^{-9} \text{ m/nm})} = 8.79 \times 10^{-19} \text{ J}
\]

\[
= (8.79 \times 10^{-19} \text{ J}) \left[ \frac{1 \text{ eV}}{1.60 \times 10^{-19} \text{ J}} \right] = 5.5 \text{ eV}
\]

2.17 A hydrogen atom exists with its electron in the n = 4 state. The electron undergoes a transition to the n = 3 state. Calculate (a) the energy of the photon emitted, (b) its frequency, and (c) its wavelength in nanometers (nm).

(a) Photon energy emitted is:

\[
\Delta E = \Delta \left[ \frac{-13.6}{n^2} \right] = \left[ \frac{-13.6}{4^2} \right] - \left[ \frac{-13.6}{3^2} \right] = 0.66 \text{ eV} = 1.06 \times 10^{-19} \text{ J}
\]

(b) Photon frequency is found as:

\[
\nu = \frac{\Delta E}{h} = \frac{1.06 \times 10^{-19} \text{ J}}{6.63 \times 10^{-34} \text{ J} \cdot \text{s}} = 1.6 \times 10^{14} \text{ Hz}
\]

(c) The wavelength is given as:

\[
\lambda = \frac{hc}{\Delta E} = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})(3.00 \times 10^8 \text{ m/s})}{(1.06 \times 10^{-19} \text{ J})(10^{-9} \text{ m/nm})} = 1876 \text{ nm}
\]

2.18 A hydrogen atom exists with its electron in the n = 6 state. The electron undergoes a transition to the n = 2 state. Calculate (a) the energy of the photon emitted, (b) its frequency, and (c) its wavelength in nanometers.

(a) Photon energy emitted is:

\[
\Delta E = \Delta \left[ \frac{-13.6}{n^2} \right] = \left[ \frac{-13.6}{6^2} \right] - \left[ \frac{-13.6}{2^2} \right] = 3.02 \text{ eV} = 4.84 \times 10^{-19} \text{ J}
\]

(b) Photon frequency is found as:
\[ \nu = \frac{\Delta E}{h} = \frac{4.84 \times 10^{-19} \text{ J}}{6.63 \times 10^{-34} \text{ J} \cdot \text{s}} = 7.3 \times 10^{14} \text{ Hz} \]

(c) The wavelength is given as:
\[ \lambda = \frac{hc}{\Delta E} = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})(3.00 \times 10^8 \text{ m/s})}{(4.84 \times 10^{-19} \text{ J})(10^{-9} \text{ m/nm})} = 410 \text{ nm} \]

2.19 In a commercial x-ray generator, a stable metal such as copper (Cu) or tungsten (W) is exposed to an intense beam of high-energy electrons. These electrons cause ionization events in the metal atoms. When the metal atoms regain their ground state, they emit x-rays of characteristic energy and wavelength. For example, a “tungsten” atom struck by a high-energy electron may lose one of its K shell electrons. When this happens, another electron, probably from the tungsten L shell will “fall” into the vacant site in the K shell. If such a \(2p \rightarrow 1s\) transition occurs in tungsten, a tungsten K\(\alpha\) x-ray is emitted. A tungsten K\(\alpha\) x-ray has a wavelength \(\lambda\) of 0.02138 nm. What is its energy? What is its frequency?

\[ E = \frac{hc}{\lambda} = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})(3.00 \times 10^8 \text{ m/s})}{(0.02138 \text{ nm})(10^{-9} \text{ m/nm})} = 9.30 \times 10^{-15} \text{ J} \]
\[ \nu = \frac{E}{h} = \frac{9.30 \times 10^{-15} \text{ J}}{6.63 \times 10^{-34} \text{ J} \cdot \text{s}} = 1.40 \times 10^{19} \text{ Hz} \]

2.20 Most modern scanning electron microscopes (SEM) are equipped with energy dispersive x-ray detectors for the purpose of chemical analysis of the specimens. This x-ray analysis is a natural extension of the capability of the SEM because the electrons that are used to form the image are also capable of creating characteristic x-rays in the sample. When the electron beam hits the specimen, x-rays specific to the elements in the specimen are created. These can be detected and used to deduce the composition of the specimen from the well-known wavelengths of the characteristic x-rays of the elements. For example:

<table>
<thead>
<tr>
<th>Element</th>
<th>Wavelength of K(\alpha) x-rays</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cr</td>
<td>0.2291 nm</td>
</tr>
<tr>
<td>Mn</td>
<td>0.2103 nm</td>
</tr>
<tr>
<td>Fe</td>
<td>0.1937 nm</td>
</tr>
<tr>
<td>Co</td>
<td>0.1790 nm</td>
</tr>
<tr>
<td>Ni</td>
<td>0.1659 nm</td>
</tr>
<tr>
<td>Cu</td>
<td>0.1542 nm</td>
</tr>
<tr>
<td>Zn</td>
<td>0.1436 nm</td>
</tr>
</tbody>
</table>
Suppose a metallic alloy is examined in an SEM and three different x-ray energies are detected. If the three energies are 7492, 5426, and 6417 eV, what elements are present in the sample? What would you call such an alloy? (Look ahead to Chap. 9 of the textbook.)

The elements may be identified by calculating their respective wavelengths.

(a) \[ \lambda = \frac{hc}{E} = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})(3.00 \times 10^8 \text{ m/s})}{(7492 \text{ eV})(1.60 \times 10^{-19} \text{ J/eV})} \]
\[ = 1.659 \times 10^{-10} \text{ m} = 0.1659 \text{ nm} \implies \text{Ni} \]

From the table provided, a wavelength of 0.1659 nm corresponds to nickel, Ni.

(b) \[ \lambda = \frac{hc}{E} = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})(3.00 \times 10^8 \text{ m/s})}{(5426 \text{ eV})(1.60 \times 10^{-19} \text{ J/eV})} \]
\[ = 2.291 \times 10^{-10} \text{ m} = 0.2291 \text{ nm} \implies \text{Cr} \]

From the table provided, a wavelength of 0.2291 nm corresponds to chromium, Cr.

(c) \[ \lambda = \frac{hc}{E} = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})(3.00 \times 10^8 \text{ m/s})}{(6417 \text{ eV})(1.60 \times 10^{-19} \text{ J/eV})} \]
\[ = 1.937 \times 10^{-10} \text{ m} = 0.1937 \text{ nm} \implies \text{Fe} \]

From the table provided, a wavelength of 0.1937 nm corresponds to iron, Fe.

The elements present, nickel, chromium, and iron, are the primary constituents of the austenitic stainless steels.

2.21 Describe the Bohr model of the hydrogen atom. What are the major shortcomings of the Bohr model?

The Bohr model of the hydrogen atom envisions an electron revolving around a proton in a circular orbit having a radius of 0.05 nm. The electron is now believed to have noncircular or elliptical orbits around the hydrogen nucleus; these were not postulated in the original Bohr theory. The exact position of the hydrogen electron at any instant cannot be precisely determined because the electron is such a small particle. Scientists presently believe that the hydrogen electron can actually deviate to some extent in its distance from the nucleus. However, the highest probability of finding the electron in space about its nucleus is still believed to be at the Bohr radius of 0.05 nm.

2.22 What is the ionization energy in electron volts for a hydrogen atom in the ground state?

The ionization energy is given as, \[ E = \frac{-13.6 \text{ eV}}{n^2} = \frac{-13.6 \text{ eV}}{1^2} = -13.6 \text{ eV} \]
2.23 Describe the four quantum numbers of an electron and give their allowed values.

1. The principal quantum number, \( n \), indicates an electron’s main energy levels, as well as, its location in space; a high probability exists for finding an electron within the \( n \) shell. This quantum number may have positive integer values of \( n = 1, 2, 3, 4 \ldots \)

2. The subsidiary quantum number, \( l \), specifies an electron’s subenergy levels and thus the subshell values where the electron is likely to be found. The allowed values are \( l = 0, 1, 2, 3, \ldots n - 1 \). The first four of these subenergy values have corresponding letter designations of \( l = s, p, d, f \) which represent electron orbitals.

3. The magnetic quantum number, \( m_l \), describes an atomic orbital’s spatial orientation and may have integral values of \(-l\) to \(+l\).

4. The electron spin quantum number, \( m_s \), provides for two electron spin directions, clockwise and counterclockwise, which are represented by the permissible values of \(+\frac{1}{2}\) and \(-\frac{1}{2}\).

2.24 Write the electron configurations of the following elements by using \textit{spdf} notation:
(a) yttrium, (b) hafnium, (c) samarium, (d) rhenium.

(a) Y (\( Z = 39 \)): \([\text{Kr}] \ 4d^15s^2 \)  
(b) Hf (\( Z = 72 \)): \([\text{Xe}] \ 4f^{14}5d^26s^2 \)  
(c) Sm (\( Z = 62 \)): \([\text{Xe}] \ 4f^66s^2 \)  
(d) Re (\( Z = 75 \)): \([\text{Xe}] \ 4f^{14}5d^56s^2 \)

2.25 What is the outer electron configuration for all the noble gases except helium? \( s^2p^6 \)

2.26 Of the noble gases Ne, Ar, Kr, and Xe, which should be the most chemically reactive?

Xenon should be most reactive since its outermost electrons (\( 5s^26p^6 \)) are further away from the nucleus than the other noble gases, and thus easier to remove.

2.27 Define the term \textit{electronegativity}.

Electronegativity is the degree to which an atom attracts electrons to itself.

2.28 Which five elements are the most electropositive according to the electronegativity scale?

The most electropositive elements are: Fr, Cs, Rb, K, Ra, and Ba. All of these have the lowest electronegativity value of 0.9.

2.29 Which five elements are the most electronegative according to the electronegativity scale?

The most electronegative elements, based on the electronegativity scale of 0 to 4.1, are: F (4.1); O (3.5); N (3.1); Cl (2.9); and Br (2.8).
2.30 Write the electron configuration of the following ions by using \textit{spdf} notation:
(a) \(\text{Cr}^{2+}, \text{Cr}^{3+}, \text{Cr}^{6+}\); (b) \(\text{Mo}^{3+}, \text{Mo}^{4+}, \text{Mo}^{6+}\), (c) \(\text{Se}^{4+}, \text{Se}^{6+}, \text{Se}^{2–}\)

(a) \(\text{Cr} [\text{Ar}] 3d^5 4s^1\)  
(b) \(\text{Mo} [\text{Kr}] 4d^5 5s^1\)  
(c) \(\text{Se} [\text{Ar}] 3d^{10} 4s^2 4p^4\)

\(\text{Cr}^{2+} [\text{Ar}] 3d^4\)  
\(\text{Mo}^{3+} [\text{Kr}] 4d^3\)  
\(\text{Se}^{4+} [\text{Ar}] 3d^{10} 4s^2\)

\(\text{Cr}^{3+} [\text{Ar}] 3d^3\)  
\(\text{Mo}^{4+} [\text{Kr}] 4d^2\)  
\(\text{Se}^{6+} [\text{Ar}] 3d^{10}\)

\(\text{Cr}^{6+} [\text{Ar}]\)  
\(\text{Mo}^{6+} [\text{Kr}] 4d^3\)  
\(\text{Se}^{2–} [\text{Ar}] 3d^{10} 4s^2 4p^6\)

2.31 Briefly describe the following types of primary bonding: (a) ionic, (b) covalent, and (c) metallic.

(a) Ionic bonding arises from the electrostatic attraction between oppositely charged ions. In the process of ion formation, an electron or a number of electrons may be transferred from a highly electropositive element to a highly electronegative one. The ionic bond in solids is nondirectional.

(b) Covalent bonding is a primary type of bonding which arises from the reduction in energy associated with the overlapping of half-filled orbitals of two atoms. In this bond, there is an electron exchange interaction. The covalent bond is a directional type of bond.

(c) Metallic bonding is a primary type of bonding involving the interaction of the valence electron or electrons of one atom with many surrounding atoms. This interaction leads to a reduction in energy of the system considered. The valence bonding electrons of these bonds are sometimes regarded as an “electron gas” bonding the positive ion cores (atoms less their valence electrons) of atoms. The metallic bond is nondirectional.

2.32 Briefly describe the following types of secondary bonding: (a) fluctuating dipole, and (b) permanent dipole.

(a) Fluctuating dipole bonding is a secondary type of bonding between atoms which contain electric dipoles. These electric dipoles, formed due to the asymmetrical electron charge distribution within the atoms, change in both direction and magnitude with time. This type of bond is electrostatic in nature, very weak and nondirectional.

(b) Permanent dipole bonding is also a secondary type of bonding between molecules possessing permanent electric dipoles. The bonds, formed by the electrostatic attraction of the dipoles, are directional in nature.

2.33 In general, why does bonding between atoms occur?

Bonding between atoms generally occurs because the atoms’ energies are lowered through the bonding process.

2.34 Describe the ionic bonding process between a pair of Na and Cl atoms. Which electrons
are involved in the bonding process?

The ionic bonding process between a pair of Na and Cl atoms involves a transfer of the outer \(3s^1\) electron of the Na atom to the \(3p\) vacancy in the Cl atom. Thus, the Na ion formed has the Ne electron configuration while the Cl ion has the Kr electron configuration.

2.35 After ionization, why is the sodium ion smaller than the sodium atom?

After ionization to the \(Na^+\), the Na atom becomes smaller because the electron-to-proton ratio of the Na atom is decreased when the \(Na^+\) ion forms. Also, the outer third shell no longer exists once the \(3s^1\) electron is lost by the Na atom.

2.36 After ionization, why is the chloride ion larger than the chlorine atom?

After ionization, the \(Cl^-\) ion is larger because the electron-to-proton ratio of the chlorine atom is decreased by the ionization process.

2.37 Calculate the attractive force \(F_{\text{attractive}}\) between a pair of \(K^+\) and \(Br^-\) ions that just touch each other. Assume the ionic radius of the \(K^+\) ion to be 0.133 nm and that of the \(Br^-\) ion to be 0.196 nm.

The attractive force between the ion pair is found by applying Coulomb’s law,

\[
F_{\text{attractive}} = \frac{-Z_1Z_2e^2}{4\pi\varepsilon_0a_o^2}
\]

Where \(Z_1 = +1\) for \(K^+\), \(Z_2 = -1\) for \(Br^-\), and \(a_o = r_{K^+} + r_{Br^-} = 0.133\ \text{nm} + 0.196\ \text{nm} = 0.329\ \text{nm} = 3.29\times10^{-10}\ \text{m}\)

Substituting,

\[
F_{\text{attractive}} = \frac{- (+1)(-1)(1.60\times10^{-19}\ \text{C})^2}{4\pi(8.85\times10^{-12}\ \text{C}^2/N\cdot\text{m}^2)(3.29\times10^{-10}\ \text{m})^2} = 2.13\times10^{-9}\ \text{N}
\]

2.38 Calculate the attractive force \(F_{\text{attractive}}\) between a pair of \(Ba^{2+}\) and \(S^{2-}\) ions that just touch each other. Assume the ionic radius of the \(Ba^{2+}\) ion to be 0.143 nm and that of the \(S^{2-}\) ion to be 0.174 nm.

The attractive force between the ion pair is found by applying Coulomb’s law,

\[
F_{\text{attractive}} = \frac{-Z_1Z_2e^2}{4\pi\varepsilon_0a_o^2}
\]

Where \(Z_1 = +2\) for \(Ba^{2+}\), \(Z_2 = -2\) for \(S^{2-}\), and
\[ a_o = r_{Ba^{2+}} + r_{S^{2-}} = 0.143 \text{ nm} + 0.174 \text{ nm} = 0.317 \text{ nm} = 3.17 \times 10^{-10} \text{ m} \]

Substituting,

\[ F_{\text{attractive}} = \frac{-(+2)(-2)(1.60 \times 10^{-19} \text{ C})^2}{4\pi(8.85 \times 10^{-12} \text{ C}^2 / \text{N} \cdot \text{m}^2)(3.17 \times 10^{-10} \text{ m})^2} = 9.16 \times 10^{-9} \text{ N} \]

2.39 Calculate the net potential energy for a K\(^+\)Br\(^-\) pair by using the \(b\) constant calculated from Problem 2.37. Assume \(n = 9.5\).

The repulsive energy constant \(b\) is:

\[ b = \frac{-F_{\text{Repulsive}}a_o^{n+1}}{n} = \frac{-(F_{\text{Attractive}})a_o^{n+1}}{n} = \frac{-(2.13 \times 10^{-9} \text{ N})(3.29 \times 10^{-10} \text{ m})^{10.5}}{9.5} \]

\[ = 6.042 \times 10^{-110} \text{ N} \cdot \text{m}^{10} \]

Thus the net potential energy between the ions is,

\[ E_{K^+Br^-} = +Z_1Z_2e^2 + \frac{b}{4\pi\varepsilon_o a_o} = + (+1)(-1)(1.60 \times 10^{-19} \text{ C})^2 + \frac{6.042 \times 10^{-110} \text{ N} \cdot \text{m}^{10}}{(3.29 \times 10^{-10} \text{ m})^{9.5}} \]

\[ = (-6.997 \times 10^{-19} \text{ J}) + (7.38 \times 10^{-20} \text{ J}) = -6.26 \times 10^{-19} \text{ J} \]

2.40 Calculate the net potential energy for a Ba\(^{2+}\)S\(^{2-}\) ion pair by using the \(b\) constant calculated from Problem 2.38. Assume \(n = 10.5\).

The repulsive energy constant \(b\) is:

\[ b = \frac{-F_{\text{Repulsive}}a_o^{n+1}}{n} = \frac{-(F_{\text{Attractive}})a_o^{n+1}}{n} = \frac{-(9.16 \times 10^{-9} \text{ N})(3.17 \times 10^{-10} \text{ m})^{11.5}}{10.5} \]

\[ = 5.045 \times 10^{-119} \text{ N} \cdot \text{m}^{10} \]

Thus the net potential energy between the ions is,

\[ E_{Ba^{2+}S^{2-}} = +Z_1Z_2e^2 + \frac{b}{4\pi\varepsilon_o a_o} = + (+2)(-2)(1.60 \times 10^{-19} \text{ C})^2 + \frac{5.045 \times 10^{-119} \text{ N} \cdot \text{m}^{10}}{(3.17 \times 10^{-10} \text{ m})^{10.5}} \]

\[ = (-2.905 \times 10^{-18} \text{ J}) + (2.765 \times 10^{-19} \text{ J}) = -2.63 \times 10^{-18} \text{ J} \]

2.41 If the attractive force between a pair of Cs\(^+\) and I\(^-\) ions is \(2.83 \times 10^{-9} \text{ N}\) and the ionic
radius of the Cs\(^+\) ion is 0.165 nm, calculate the ionic radius of the I\(^-\) ion in nanometers.

From Coulomb’s law,

\[
a_o = \frac{1}{4\pi \varepsilon_o F_{\text{Attractive}}} = \frac{1}{4\pi (8.85 \times 10^{-12} \text{ C}^2/(\text{N} \cdot \text{m}^2))(2.83 \times 10^{-9} \text{ N})} = 2.852 \times 10^{-10} \text{ m} = 0.2852 \text{ nm}
\]

The ionic radius of iodine is thus,

\[
r_{\text{I}^-} = a_o - r_{\text{Cs}^+} = 0.285 \text{ nm} - 0.165 \text{ nm} = 0.120 \text{ nm}
\]

2.42 If the attractive force between a pair of Sr\(^{2+}\) and O\(^{2-}\) ions is \(1.29 \times 10^{-8} \text{ N}\) and the ionic radius of the O\(^{2-}\) ion is 0.132 nm, calculate the ionic radius of the Sr\(^{2+}\) ion in nanometers.

From Coulomb’s law,

\[
a_o = \frac{1}{4\pi \varepsilon_o F_{\text{Attractive}}} = \frac{1}{4\pi (8.85 \times 10^{-12} \text{ C}^2/(\text{N} \cdot \text{m}^2))(1.29 \times 10^{-8} \text{ N})} = 2.672 \times 10^{-10} \text{ m} = 0.2672 \text{ nm}
\]

The ionic radius of iodine is thus,

\[
r_{\text{Sr}^{2+}} = a_o - r_{\text{O}^{2-}} = 0.267 \text{ nm} - 0.132 \text{ nm} = 0.135 \text{ nm}
\]

2.43 Describe the two major factors that must be taken into account in the packing of ions in an ionic crystal.

1. The structure of ionic solids is partly determined by the radii of the cations and anions of the ionic solid. Only certain ranges of cation-to-anion radius ratios are allowed by packing considerations.

2. Electrical neutrality must be maintained. Thus, if the cations and anions have different valences, the number of anions surrounding a particular cation will be restricted.

2.44 Describe the covalent bonding process between a pair of hydrogen atoms. What is the driving energy for the formation of a diatomic molecule?

The covalent bonding in the hydrogen molecule involves the interaction and overlapping of the 1s orbitals of the hydrogen atoms. The covalent bond forms between the two hydrogen atoms because their energies are lowered by the bonding process.

2.45 Describe the covalent bonding electron arrangement in the following diatomic molecules: (a) fluorine, (b) oxygen, (c) nitrogen.

(a) In fluorine molecules, a single covalent bond is formed between the \(p\) orbitals of two
fluorine atoms.

(b) In oxygen molecules, a double covalent bond is formed between the $p$ orbitals of two oxygen atoms.

(c) In nitrogen molecules, a triple covalent bond is formed between the $p$ orbitals of two nitrogen atoms.

2.46 Describe the hybridization process for the formation of four equivalent $sp^3$ hybrid orbitals in carbon during covalent bonding. Use orbital diagrams.

In the hybridization process, four equal $sp^3$ hybrid orbitals are formed in the carbon atom. This is accomplished through the promotion of one of the 2s orbitals to a 2p level.

2.47 List the number of atoms bonded to a C atom that exhibits $sp^3$, $sp^2$, and $sp$ hybridization. For each, give the geometrical arrangement of the atoms in the molecule.

- $sp^3$ hybridization: Four atoms are bonded to a central carbon atom in a tetrahedral arrangement. An example is methane, CH$_4$.
- $sp^2$ hybridization: Three atoms are bonded to a carbon atom in a planar arrangement. An example is ethylene, CH$_2$: CH$_2$.
- $sp$ hybridization: Two atoms are bonded to a carbon atom in a linear arrangement. An example is acetylene, CH:CH.

Diamond is extremely hard because its carbon atoms are covalently bonded by single $sp^3$ hybrid bonds in a three dimensional arrangement.

2.49 Describe the metallic bonding process among an aggregate of copper atoms.
Copper has a crystal structure of closely packed atoms; each atom is surrounded by twelve others. This compact structure is due, in part, to the fact that each atom has only one valence electron. Consequently, there is a low density electron charge cloud available for bonding.

2.50 How can the high electrical and thermal conductivities of metals be explained by the “electron gas” model of metallic bonding? Ductility?

The high electrical and thermal conductivities of metals are explained by the mobility of their outer valence electrons in the presence of an electrical potential or thermal gradient. The ductility of metals is explained by the bonding “electron gas” which enables atoms to pass over each other during deformation, without severing their bonds.

2.51 The melting point of the metal potassium is 63.5°C, while that of titanium is 1660°C. What explanation can be given for this great difference in melting temperatures?

The significantly higher melting point of titanium, as compared to potassium, is in part attributed to the hybridized covalent bonding between the 3d and 4s orbitals of titanium.

2.52 Is there a correlation between the electron configurations of the element potassium (Z = 19) through copper (Z = 29) and their melting points? (See Tables 2.8 and 2.9.)

A possible correlation between the melting points and the electron configurations of the elements from scandium (Z = 21) to copper (Z = 29) is that unpaired 3d electrons cause covalent hybridized bonds, and hence give higher melting points to these transition metals.

2.53 Using the covalent-metallitivity values of Table 2.9, calculate values for the percent metallic and covalent bonding in the structural metal titanium.

Assuming purely covalent and metallic bonding in the titanium,

\[
\% \text{ covalent bonding} = \frac{1.91}{4.00} \times 100\% = 47.75\%
\]

\[
\% \text{ metallic bonding} = 100\% - 47.75\% = 52.25\%
\]

2.54 Using the covalent-metallitivity values of Table 2.9, calculate values for the percent metallic and covalent bonding in the metal tungsten.

Assuming purely covalent and metallic bonding in the tungsten,

\[
\% \text{ covalent bonding} = \frac{3.86}{4.00} \times 100\% = 96.50\%
\]

\[
\% \text{ metallic bonding} = 100\% - 96.50\% = 3.50\%
\]
2.55 Define an electric dipole moment.

An electric dipole moment is defined as the product of the absolute charge of one of the dipoles (positive or negative) multiplied by the separation distance between the positive and negative dipole charges.

2.56 Describe fluctuating dipole bonding among the atoms of the noble gas neon. Of a choice between the noble gases krypton and xenon, which noble gas would be expected to have the strongest dipole bonding and why?

A fluctuating electric dipole exists in the atoms of noble gases, such as neon, because there is, at any instant, an asymmetrical distribution of electrical charge among their electrons. The noble gas xenon would be expected to have a stronger fluctuating dipole moment than krypton since it has an additional electron shell; the krypton atom has four electron shells while the xenon atom has five. The electrons of this fifth shell, being further away from the xenon nucleus, and are able to fluctuate more and thus create greater asymmetry of charge.

2.57 Describe permanent dipole bonding among polar covalent molecules.

Polar covalent molecules with permanent dipoles bond together because of the electrostatic attraction of their positive and negative charge centers.

2.58 Carbon tetrachloride (CCl\(_4\)) has a zero dipole moment. What does this tell us about the C—Cl bonding arrangement in this molecule?

Since the molecule CCl\(_4\) has a zero dipole moment, the C—Cl bonding arrangement must be symmetrical about the carbon nucleus.

2.59 Describe the hydrogen bond. Among what elements is this bond restricted?

The hydrogen bond is a permanent dipole bond restricted to a hydrogen atom and highly electronegative atoms such as O, N, F and Cl. This secondary bond is relatively strong due to the small size of the hydrogen atom.

2.60 Describe hydrogen bonding among water molecules.

Hydrogen bonding occurs between water molecules because of the electrostatic attraction between the negatively charged oxygen regions of the water molecules and the positively charged hydrogen regions.

2.61 Methane (CH\(_4\)) has a much lower boiling temperature than does water (H\(_2\)O). Explain why this is true in terms of the bonding between molecules in each of these two substances.
The methane molecules are bonded together by weak –C–H dipoles. The water molecules are bonded together by the much stronger –O–H hydrogen bonded dipoles.

2.62 Sketch a tetrahedron and make a small model of one from cardboard and tape with a 2-inch side. Do the same for an octahedron.

The models should resemble these 3-D sketches:

![Tetrahedron](image1.png) ![Octahedron](image2.png)

2.63 What is Pauling’s equation for determining the percentage ionic character in a mixed ionic-covalently bonded compound?

Pauling’s equation relating the percent ionic character of an ionic-covalent bond to the electronegativites of the bonding atoms is:

\[
\text{% Ionic Character} = [1 - e^{-0.25(x_a - x_b)^2}] \times 100\%
\]

where \(x_A\) is the electronegativity of the more electropositive element and \(x_B\) is the electronegativity of the more electronegative element.

2.64 Compare the percentage ionic character in the semiconducting compound CdTe and InP.

Applying Pauling’s equation to CdTe and InP compounds,

For CdTe (2 – 6), \(\text{% Ionic character} = (1 - e^{-0.25(1.5-2.0)^2})(100\%) = 6.1\%\)

For InP (3 – 5), \(\text{% Ionic character} = (1 - e^{-0.25(1.5-2.1)^2})(100\%) = 8.6\%\)

While a 2 – 6 compound typically has a higher ionic character than a 3 – 5, the relatively high electronegativity of phosphorous causes InP to be more ionic in nature.

2.65 Compare the percentage ionic character in the semiconducting compound InSb and ZnTe.

Applying Pauling’s equation to InSb and ZnTe compounds,

For InSb (2 – 6), \(\text{% Ionic character} = (1 - e^{-0.25(1.5-1.8)^2})(100\%) = 2.2\%\)

For ZnTe (3 – 5), \(\text{% Ionic character} = (1 - e^{-0.25(1.7-2.0)^2})(100\%) = 2.2\%\)

While a 2 – 6 compound typically has a higher ionic character than a 3 – 5, in this case, the compounds have identical ionic character.
For each of the following compounds, state whether the bonding is essentially metallic, covalent, ionic, van der Waals, or hydrogen: (a) Ni, (b) ZrO₂, (c) graphite, (d) solid Kr, (e) Si, (f) BN, (g) SiC, (h) Fe₂O₃, (i) MgO, (j) W, (k) H₂O within the molecules, (l) H₂O between the molecules.

If ionic and covalent bonding are involved in the bonding of any of the compounds listed, calculate the percentage ionic character in the compound.

(a) Ni: Nickel bonding is primarily metallic.
(b) ZrO₂: From Pauling’s equation, the Zr–O bond is 73.4% ionic and 26.6% covalent, where \( x_A \) and \( x_B \) are the electronegativities of zirconium and oxygen, respectively.
(c) Graphite: The bonding is covalent within the layers and secondary between the layers.
(d) Solid Kr: The bonding represents van der Waals due to fluctuating dipoles.
(e) Si: Silicon bonding is covalent.
(f) BN: The B–N bond, from Pauling’s equation (2-10), is 26.1% ionic and 73.9% covalent.
(g) SiC: From Eq. (2-10), the Si–C bond is 11% ionic and 89% covalent.
(h) Fe₂O₃: From Eq. (2-10), the Fe–O bond is 55.5% ionic and 44.5% covalent.
(i) MgO: From Eq. (2-10), the Mg–O bond is 70.2% ionic and 29.8% covalent.
(j) W: Tungsten bonding primarily consists of metallic bonding with some covalent character.
(k) H₂O within the molecules: The H–O bond is 38.7% ionic and 61.3% covalent.
(l) H₂O between the molecules: Hydrogen bonding exists between H₂O molecules.
CHAPTER 3  ATOMIC STRUCTURE AND BONDING

3.1 Define a crystalline solid.

A crystalline solid is one which has a crystal structure in which atoms or ions are arranged in a pattern that repeats itself in three dimensions.

3.2 Define a crystal structure. Give examples of materials which have crystal structures.

A crystal structure is identical to a crystalline solid, as defined by the solution of Problem 3.1. Examples include metals, ionic crystals and certain ceramic materials.

3.3 Define a space lattice.

A space lattice is an infinite three-dimensional array of points with each point having identical surrounding points.

3.4 Define a unit cell of a space lattice. What lattice constants define a unit cell?

The unit cell of a space lattice represents a repeating unit of atomic spatial positions. The cell is defined by the magnitudes and directions of three lattice vectors, \( \mathbf{a} \), \( \mathbf{b} \), and \( \mathbf{c} \): axial lengths \( a \), \( b \), and \( c \); interaxial angles \( \alpha \), \( \beta \), and \( \gamma \).

3.5 What are the 14 Bravais unit cells?

The fourteen Bravais lattices are: simple cubic, body-centered cubic, face-centered cubic, simple tetragonal, body-centered tetragonal, simple orthorhombic, base-centered orthorhombic, body-centered orthorhombic, face-centered orthorhombic, simple rhombohedral, simple hexagonal, simple monoclinic, base-centered monoclinic, and simple triclinic.

3.6 What are the three most common metal crystal structures? List five metals which have each of these crystal structures.

The three most common crystal structures found in metals are: body-centered cubic (BCC), face-centered cubic (FCC), and hexagonal close-packed (HCP). Examples of metals having these structures include the following.

- **BCC**: \( \alpha \)– iron, vanadium, tungsten, niobium, and chromium.
- **FCC**: copper, aluminum, lead, nickel, and silver.
- **HCP**: magnesium, \( \alpha \)– titanium, zinc, beryllium, and cadmium.

3.7 How many atoms per unit cell are there in the BCC crystal structure?
A BCC crystal structure has two atoms in each unit cell.

3.8 What is the coordination number for the atoms in the BCC crystal structure?

A BCC crystal structure has a coordination number of eight.

3.9 What is the relationship between the length of the side $a$ of the BCC unit cell and the radius of its atoms?

In a BCC unit cell, one complete atom and two atom eighths touch each other along the cube diagonal. This geometry translates into the relationship $\sqrt{3}a = 4R$.

3.10 Molybdenum at 20ºC is BCC and has an atomic radius of 0.140 nm. Calculate a value for its lattice constant $a$ in nanometers.

Letting $a$ represent the edge length of the BCC unit cell and $R$ the molybdenum atomic radius,

$$\sqrt{3}a = 4R \quad \text{or} \quad a = \frac{4}{\sqrt{3}} R = \frac{4}{\sqrt{3}} (0.140 \text{ nm}) = \textbf{0.323 nm}$$

3.11 Niobium at 20ºC is BCC and has an atomic radius of 0.143 nm. Calculate a value for its lattice constant $a$ in nanometers.

For a BCC unit cell having an edge length $a$ and containing niobium atoms,

$$\sqrt{3}a = 4R \quad \text{or} \quad a = \frac{4}{\sqrt{3}} R = \frac{4}{\sqrt{3}} (0.143 \text{ nm}) = \textbf{0.330 nm}$$

3.12 Lithium at 20ºC is BCC and has an atomic radius of 0.35092 nm. Calculate a value for the atomic radius of a lithium atom in nanometers.

For the lithium BCC structure, which has a lattice constant of $a = 0.35092$ nm, the atomic radius is,

$$R = \frac{\sqrt{3}}{4} a = \frac{\sqrt{3}}{4} (0.35092 \text{ nm}) = \textbf{0.152 nm}$$

3.13 Sodium at 20ºC is BCC and has an atomic radius of 0.42906 nm. Calculate a value for the atomic radius of sodium atom in nanometers.

For the sodium BCC structure, with a lattice constant of $a = 0.42906$ nm, the atomic radius is,
3.14 How many atoms per unit cell are there in the FCC crystal structure?

Each unit cell of the FCC crystal structure contains four atoms.

3.15 What is the coordination number for the atoms in the FCC crystal structure?

The FCC crystal structure has a coordination number of twelve.

3.16 Gold is FCC and has a lattice constant of 0.40788 nm. Calculate a value for the atomic radius of a gold atom in nanometers.

For the gold FCC structure, which has a lattice constant of \( a = 0.40788 \) nm, the atomic radius is,

\[
R = \frac{\sqrt{2}}{4}a = \frac{\sqrt{2}}{4}(0.40788 \text{ nm}) = 0.144 \text{ nm}
\]

3.17 Platinum is FCC and has a lattice constant of 0.39239 nm. Calculate a value for the atomic radius of a platinum atom in nanometers.

For the platinum FCC structure, with a lattice constant of \( a = 0.39239 \) nm, the atomic radius is,

\[
R = \frac{\sqrt{2}}{4}a = \frac{\sqrt{2}}{4}(0.39239 \text{ nm}) = 0.139 \text{ nm}
\]

3.18 Palladium is FCC and has an atomic radius of 0.137 nm. Calculate a value for its lattice constant \( a \) in nanometers.

Letting \( a \) represent the FCC unit cell edge length and \( R \) the palladium atomic radius,

\[
\sqrt{2}a = 4R \quad \text{or} \quad a = \frac{4}{\sqrt{2}}R = \frac{4}{\sqrt{2}}(0.137 \text{ nm}) = 0.387 \text{ nm}
\]

3.19 Strontium is FCC and has an atomic radius of 0.215 nm. Calculate a value for its lattice constant \( a \) in nanometers.

For an FCC unit cell having an edge length \( a \) an containing strontium atoms,

\[
\sqrt{2}a = 4R \quad \text{or} \quad a = \frac{4}{\sqrt{2}}R = \frac{4}{\sqrt{2}}(0.215 \text{ nm}) = 0.608 \text{ nm}
\]
3.20 Calculate the atomic packing factor for the FCC structure.

By definition, the atomic packing factor is given as:

\[
\text{Atomic packing factor} = \frac{\text{volume of atoms in FCC unit cell}}{\text{volume of the FCC unit cell}}
\]

These volumes, associated with the four-atom FCC unit cell, are

\[
V_{\text{atoms}} = 4 \left( \frac{4}{3} \pi R^3 \right) = \frac{16}{3} \pi R^3 \quad \text{and} \quad V_{\text{unit cell}} = a^3
\]

where \(a\) represents the lattice constant. Substituting \(a = \frac{4R}{\sqrt{2}}\),

\[
V_{\text{unit cell}} = a^3 = \frac{64R^3}{2\sqrt{2}}
\]

The atomic packing factor then becomes,

\[
\text{APF (FCC unit cell)} = \frac{16\pi R^3}{3} \left( \frac{1}{32R^3} \right) = \frac{\pi \sqrt{2}}{6} = 0.74
\]

3.21 How many atoms per unit cell are there in the HCP crystal structure?

The hexagonal prism contains six atoms.

3.22 What is the coordination number for the atoms in the HCP crystal structure?

The coordination number associated with the HCP crystal structure is twelve.

3.23 What is the ideal \(c/a\) ratio for HCP metals?

The ideal \(c/a\) ratio for HCP metals is 1.633; however, the actual ratios may deviate significantly from this value.

3.24 Of the following HCP metals, which have higher or lower \(c/a\) ratios than the ideal ratio: Zr, Ti, Zn, Mg, Co, Cd and Be?

Cadmium and zinc have significantly higher \(c/a\) ratios while zirconium, titanium, magnesium, cobalt and beryllium have slightly lower ratios.

3.25 Calculate the volume in cubic nanometers of the titanium crystal structure unit cell. Titanium is HCP at 20ºC with \(a = 0.29504\) nm and \(c = 0.46833\) nm.

For a hexagonal prism, of height \(c\) and side length \(a\), the volume is given by:
\[ V = (\text{Area of Base})(\text{Height}) = [(6 \times \text{Equilateral Triangle Area})(\text{Height})] \]
\[ = (3a^2 \sin 60^\circ)(c) \]
\[ = 3(0.29504 \text{ nm})^2(\sin 60^\circ)(0.46833 \text{ nm}) \]
\[ = 0.106 \text{ nm}^3 \]

3.26  Rhenium at 20ºC is HCP. The height \( c \) of its unit cell is 0.44583 nm and its \( c/a \) ratio is 1.633 nm. Calculate a value for its lattice constant \( a \) in nanometers.

The rhenium lattice constant \( a \) is calculated as,
\[ a = \frac{c}{c/a} = \frac{0.44583 \text{ nm}}{1.633} = 0.273 \text{ nm} \]

3.27  Osmium at 20ºC is HCP. Using a value of 0.135 nm for the atomic radius of osmium atoms, calculate a value for its unit-cell volume. Assume a packing factor of 0.74.

From the definition of the atomic packing factor,
\[ \text{HCP unit cell volume} = \frac{\text{volume of atoms in HCP unit cell}}{\text{APF}} \]

Since there are six atoms in the HCP unit cell, the volume of atoms is:
\[ V_{\text{atoms}} = 6 \left( \frac{4}{3} \pi R^3 \right) = 8 \pi (0.135)^3 = 0.0618 \text{ nm}^3 \]

The unit cell volume thus becomes,
\[ \text{HCP unit cell volume} = \frac{0.0618 \text{ nm}^3}{0.74} = 0.084 \text{ nm}^3 \]

3.28  How are atomic positions located in cubic unit cells?

Atomic positions are located in cubic unit cells using rectangular \( x, y, \) and \( z \) axes and unit distances along the respective axes. The directions of these axes are shown below.
3.29 List the atom positions for the eight corner and six face-centered atoms of the FCC unit cell.

The atom positions at the corners of an FCC unit cell are:

\((0, 0, 0), (1, 0, 0), (1, 1, 0), (0, 1, 0), (0, 0, 1), (1, 0, 1), (1, 1, 1), (0, 1, 1)\)

On the faces of the FCC unit cell, atoms are located at:

\((½, ½, 0), (½, 0, ½), (0, ½, ½), (½, ½, 1), (1, ½, ½), (½, 1, ½)\)

3.30 How are the indices for a crystallographic direction in a cubic unit cell determined?

For cubic crystals, the crystallographic direction indices are the components of the direction vector, resolved along each of the coordinate axes and reduced to the smallest integers. These indices are designated as \([uvw]\).

3.31 Draw the following directions in a BCC unit cell and list the position coordinates of the atoms whose centers are intersected by the direction vector:

(a) \([100]\)  
(b) \([110]\)  
(c) \([111]\)

(a) Position Coordinates: \((0, 0, 0), (1, 0, 0)\)  
(b) Position Coordinates: \((0, 0, 0), (1, 1, 0)\)  
(c) Position Coordinates: \((0, 0, 0), (1, 1, 1)\)

3.32 Draw direction vectors in unit cubes for the following cubic directions:

(a) \([11\bar{1}]\)  
(b) \([1\bar{1}0]\)  
(c) \([\bar{1}2\bar{1}]\)  
(d) \([\bar{1}\bar{1}3]\)
3.33 Draw direction vectors in unit cubes for the following cubic directions:

(a) \([\bar{1} \bar{2} 2]\)  
(b) \([1 \bar{2} 3]\)  
(c) \([\bar{3} 3 1]\)  
(d) \([0 \bar{2} 1]\)  
(e) \([2 \bar{1} 2]\)  
(f) \([2 3 3]\)  
(g) \([\bar{1} 0 1]\)  
(h) \([1 2 \bar{1}\)]  
(i) \([3 2 1]\)  
(j) \([1 0 \bar{3}\)]  
(k) \([1 \bar{2} 2]\)  
(l) \([\bar{2} 2 3]\)

(a) Dividing \([\bar{1} \bar{2} 2]\) by 2,
\[x = \frac{1}{2}, \quad y = -\frac{1}{2}, \quad z = -\frac{1}{2}\]

(b) Dividing \([1 \bar{2} 3]\) by 3,
\[x = \frac{1}{3}, \quad y = -\frac{2}{3}, \quad z = 1\]

(c) Dividing \([\bar{3} 3 1]\) by 3,
\[x = -1, \quad y = 1, \quad z = \frac{1}{3}\]

(d) Dividing \([0 \bar{2} 1]\) by 2,
\[x = 0, \quad y = -1, \quad z = \frac{1}{2}\]

(e) Dividing \([2 \bar{1} 2]\) by 2,
\[x = 1, \quad y = -\frac{1}{2}, \quad z = 1\]

(f) Dividing \([2 3 3]\) by 3,
\[x = \frac{2}{3}, \quad y = -1, \quad z = 1\]
3.34 What are the indices of the directions shown in the unit cubes of Fig. P3.34?

(g) For [101],
\[ x = -1, \ y = 0, \ z = 1 \]

(h) Dividing [121] by 2,
\[ x = \frac{1}{2}, \ y = 1, \ z = -\frac{1}{2} \]

(i) Dividing [321] by 3,
\[ x = 1, \ y = \frac{2}{3}, \ z = \frac{1}{3} \]

(j) Dividing [103] by 3,
\[ x = \frac{1}{3}, \ y = 0, \ z = -1 \]

(k) Dividing [122] by 2,
\[ x = \frac{1}{2}, \ y = -1, \ z = -1 \]

(l) Dividing [223] by 3,
\[ x = -\frac{2}{3}, \ y = -\frac{2}{3}, \ z = 1 \]
a. Vector components: 
\[ x = -1, \ y = 1, \ z = 0 \]
Direction indices: \([110]\)

b. Moving direction vector down \(\frac{1}{4}\), vector components are: 
\[ x = 1, \ y = -1, \ z = \frac{1}{4} \]
Direction indices: \([441]\)

c. Moving direction vector forward \(\frac{1}{2}\), vector components are: 
\[ x = -\frac{1}{6}, \ y = 1, \ z = 1 \]
Direction indices: \([\bar{1}66]\)

d. Moving direction vector left \(\frac{1}{4}\), vector components are: 
\[ x = 1, \ y = \frac{1}{2}, \ z = 1 \]
Direction indices: \([212]\)

e. Vector components are: 
\[ x = -\frac{1}{4}, \ y = -1, \ z = 1 \]
Direction indices: \([\bar{3}44]\)

f. Moving direction vector up \(\frac{1}{3}\), vector components are: 
\[ x = -1, \ y = 1, \ z = -\frac{1}{3} \]
Direction indices: \([\bar{3}3\bar{1}]\)

g. Moving direction vector up \(\frac{1}{2}\), vector components are: 
\[ x = 1, \ y = -1, \ z = -\frac{1}{4} \]
Direction indices: \([441]\)

h. Moving direction vector up \(\frac{1}{4}\), vector components are: 
\[ x = \frac{1}{4}, \ y = -1, \ z = -\frac{1}{4} \]
Direction indices: \([3\bar{4}3]\)
3.35 A direction vector passes through a unit cube from the \( \left( \frac{3}{4}, 0, \frac{1}{4} \right) \) to the \( \left( \frac{1}{2}, 1, 0 \right) \) positions. What are its direction indices?

The starting point coordinates, subtracted from the end point, give the vector components:

\[
x = \frac{1}{2} - \frac{3}{4} = -\frac{1}{4} \quad y = 1 - 0 = 1 \quad z = 0 - \frac{1}{4} = -\frac{1}{4}
\]

The fractions can then be cleared through multiplication by 4, giving

\( x = -1, \ y = 4, \ z = -1 \). The direction indices are therefore \([\overline{1} \ 4 \ 1]\).

3.36 A direction vector passes through a unit cube from the \( (1, 0, \frac{3}{4}) \) to the \( (\frac{1}{4}, 1, \frac{1}{4}) \) positions. What are its direction indices?

Subtracting coordinates, the vector components are:

\[
x = \frac{1}{4} - 1 = -\frac{3}{4} \quad y = 1 - 0 = 1 \quad z = \frac{1}{4} - \frac{3}{4} = -\frac{1}{2}
\]

Clearing fractions through multiplication by 4, gives \( x = -3, \ y = 4, \ z = -2 \). The direction indices are therefore \([3 \ 4 \ 2]\).

3.37 What are the crystallographic directions of a family or form? What generalized notation is used to indicate them?

A family or form has equivalent crystallographic directions; the atom spacing along each direction is identical. These directions are indicated by \(\langle uvw\rangle\).

3.38 What are the directions of the \(\langle 100\rangle\) family or form for a unit cube?

\([100], [010], [001], [\overline{1} \ 0 \ 0], [0 \overline{1} \ 0], [00\overline{1}]\)

3.39 What are the directions of the \(\langle 111\rangle\) family or form for a unit cube?

\([111], [\overline{1} \ 1 \ 1], [\overline{1} \ 1 \ 0], [\overline{1} \ 1 \ 1], [\overline{1} \overline{1} \overline{1}], [\overline{1} \overline{1} \ 1], [\overline{1} \overline{1} \overline{1}]\)

3.40 What \(\langle 110\rangle\)-type directions lie on the \(\langle 111\rangle\) plane of a cubic unit cell?

\([0 \overline{1} \ 1], [0 \ 1 \ 1], [\overline{1} \ 0 \ 0], [\overline{1} \ 1 \ 0], [\overline{1} \ 0 \ 1], [0 \ 1 \ 0]\)
3.41 What \{111\}-type directions lie on the (110) plane of a cubic unit cell?

\([1\bar{1}1], [\bar{1}11], [1\bar{1}1], [1\bar{1}1]\)

3.42 How are the Miller indices for a crystallographic plane in a cubic unit cell determined? What generalized notation is used to indicate them?

The Miller indices are determined by first identifying the fractional intercepts which the plane makes with the crystallographic \(x\), \(y\), and \(z\) axes of the cubic unit cell. Then all fractions must be cleared such that the smallest set of whole numbers is attained. The general notation used to indicate these indices is \((hkl)\), where \(h\), \(k\), and \(l\) correspond to the \(x\), \(y\) and \(z\) axes, respectively.

3.43 Draw in unit cubes the crystal planes that have the following Miller indices:

(a) \((1\bar{1}1)\)  (d) \((2\bar{1}3)\)  (g) \((2\bar{1}1)\)  (j) \((1\bar{3}3)\)
(b) \((10\bar{2})\)  (e) \((3\bar{2}1)\)  (h) \((\bar{2}1\bar{2})\)  (k) \((3\bar{1}2)\)
(c) \((1\bar{2}1)\)  (f) \((3\bar{0}2)\)  (i) \((\bar{2}3\bar{2})\)  (l) \((\bar{3}\bar{3}\bar{1})\)

a. For \((1\bar{1}1)\) reciprocals are: \(x = 1\), \(y = -1\), \(z = -1\)
b. For \((10\bar{2})\) reciprocals are: \(x = 1\), \(y = \infty\), \(z = -\frac{1}{2}\)
c. For \((1\bar{2}1)\) reciprocals are: \(x = 1\), \(y = -\frac{1}{2}\), \(z = -1\)
d. For \((2\bar{1}3)\) reciprocals are: \(x = \frac{1}{2}\), \(y = 1\), \(z = -\frac{1}{3}\)
e. For \((3\bar{2}1)\) reciprocals are: \(x = \frac{1}{3}\), \(y = -\frac{1}{2}\), \(z = 1\)
f. For \((3\bar{0}2)\) reciprocals are: \(x = \frac{1}{3}\), \(y = \infty\), \(z = -\frac{1}{2}\)
3.44 What are the Miller indices of the cubic crystallographic planes shown in Fig. P3.44?

g. For (201) reciprocals are: \(x = \frac{1}{2}, y = \infty, z = -1\)

h. For (212) reciprocals are: \(x = -\frac{1}{2}, y = 1, z = -\frac{1}{2}\)

i. For (232) reciprocals are: \(x = -\frac{1}{2}, y = \frac{1}{2}, z = \frac{1}{2}\)

j. For (133) reciprocals are: \(x = 1, y = \frac{1}{3}, z = -\frac{1}{3}\)

k. For (312) reciprocals are: \(x = -\frac{1}{3}, y = -1, z = \frac{1}{2}\)

k. For (331) reciprocals are: \(x = -\frac{1}{3}, y = \frac{1}{3}, z = -1\)
### Miller Indices for Figure P3.44(a)

<table>
<thead>
<tr>
<th>Plane a based on (0, 1, 1) as origin</th>
<th>Plane b based on (1, 1, 0) as origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Planar Intercepts</td>
<td>Planar Intercepts</td>
</tr>
<tr>
<td>Reciprocals of Intercepts</td>
<td>Reciprocals of Intercepts</td>
</tr>
<tr>
<td>( x = \infty )</td>
<td>( x = -1 )</td>
</tr>
<tr>
<td>( \frac{1}{x} = 0 )</td>
<td>( \frac{1}{x} = -1 )</td>
</tr>
<tr>
<td>( y = -1 )</td>
<td>( y = \frac{-5}{12} )</td>
</tr>
<tr>
<td>( \frac{1}{y} = -1 )</td>
<td>( \frac{1}{y} = \frac{-12}{5} )</td>
</tr>
<tr>
<td>( z = -\frac{1}{4} )</td>
<td>( z = \infty )</td>
</tr>
<tr>
<td>( \frac{1}{z} = -4 )</td>
<td>( \frac{1}{z} = 0 )</td>
</tr>
</tbody>
</table>

The Miller indices of plane a are (0 1 4).
The Miller indices of plane b are (5 12 0).

<table>
<thead>
<tr>
<th>Plane c based on (1, 1, 0) as origin</th>
<th>Plane d based on (0, 0, 0) as origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Planar Intercepts</td>
<td>Planar Intercepts</td>
</tr>
<tr>
<td>Reciprocals of Intercepts</td>
<td>Reciprocals of Intercepts</td>
</tr>
<tr>
<td>( x = \infty )</td>
<td>( x = 1 )</td>
</tr>
<tr>
<td>( \frac{1}{x} = 0 )</td>
<td>( \frac{1}{x} = 1 )</td>
</tr>
<tr>
<td>( y = -1 )</td>
<td>( y = 1 )</td>
</tr>
<tr>
<td>( \frac{1}{y} = -1 )</td>
<td>( \frac{1}{y} = 1 )</td>
</tr>
<tr>
<td>( z = \frac{1}{3} )</td>
<td>( z = \frac{2}{3} )</td>
</tr>
<tr>
<td>( \frac{1}{z} = 3 )</td>
<td>( \frac{1}{z} = \frac{3}{2} )</td>
</tr>
</tbody>
</table>

The Miller indices of plane c are (0 1 3).
The Miller indices of plane d are (2 2 3).

### Miller Indices for Figure P3.44(b)

<table>
<thead>
<tr>
<th>Plane a based on (1, 1, 0) as origin</th>
<th>Plane b based on (1, 1, 0) as origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Planar Intercepts</td>
<td>Planar Intercepts</td>
</tr>
<tr>
<td>Reciprocals of Intercepts</td>
<td>Reciprocals of Intercepts</td>
</tr>
<tr>
<td>( x = -1 )</td>
<td>( x = 1 )</td>
</tr>
<tr>
<td>( \frac{1}{x} = -1 )</td>
<td>( \frac{1}{x} = 1 )</td>
</tr>
<tr>
<td>( y = \infty )</td>
<td>( y = -1 )</td>
</tr>
<tr>
<td>( \frac{1}{y} = 0 )</td>
<td>( \frac{1}{y} = -1 )</td>
</tr>
<tr>
<td>( z = -\frac{1}{3} )</td>
<td>( z = -\frac{2}{3} )</td>
</tr>
<tr>
<td>( \frac{1}{z} = -3 )</td>
<td>( \frac{1}{z} = -3 )</td>
</tr>
</tbody>
</table>

The Miller indices of plane a are (1 0 3).
The Miller indices of plane b are (2 2 3).
### Plane c based on \((0, 1, 0)\) as origin

<table>
<thead>
<tr>
<th>Planar Intercepts</th>
<th>Reciprocals of Intercepts</th>
</tr>
</thead>
<tbody>
<tr>
<td>(x = 1)</td>
<td>(\frac{1}{x} = 1)</td>
</tr>
<tr>
<td>(y = \frac{-5}{12})</td>
<td>(\frac{1}{y} = \frac{-12}{5})</td>
</tr>
<tr>
<td>(z = \infty)</td>
<td>(\frac{1}{z} = 0)</td>
</tr>
</tbody>
</table>

The Miller indices of plane \(c\) are \((5\overline{12}0)\).  

### Plane d based on \((0, 1, 0)\) as origin

<table>
<thead>
<tr>
<th>Planar Intercepts</th>
<th>Reciprocals of Intercepts</th>
</tr>
</thead>
<tbody>
<tr>
<td>(x = 1)</td>
<td>(\frac{1}{x} = 1)</td>
</tr>
<tr>
<td>(y = -1)</td>
<td>(\frac{1}{y} = -1)</td>
</tr>
<tr>
<td>(z = \frac{1}{2})</td>
<td>(\frac{1}{z} = 2)</td>
</tr>
</tbody>
</table>

The Miller indices of plane \(d\) are \((1\overline{1}2)\).  

3.45 What is the notation used to indicate a family or form of cubic crystallographic planes?  
A family or form of a cubic crystallographic plane is indicated using the notation \(\{hkl\}\).  

3.46 What are the \(\{100\}\) family of planes of the cubic system?  
\((100), (010), (001), (\overline{1}00), (0\overline{1}0), (00\overline{1})\)  

3.47 Draw the following crystallographic planes in a BCC unit cell and list the position of the atoms whose centers are intersected by each of the planes:  
(a) \((100)\)  
(b) \((110)\)  
(c) \((111)\)

3.48 Draw the following crystallographic planes in an FCC unit cell and list the position coordinates of the atoms whose centers are intersected by each of the planes:  
(a) \((100)\)  
(b) \((110)\)  
(c) \((111)\)
3.49 A cubic plane has the following axial intercepts: \( a = \frac{1}{3}, \ b = -\frac{1}{3}, \ c = \frac{1}{2} \). What are the Miller indices of this plane?

Given the axial intercepts of \( (\frac{1}{3}, -\frac{1}{3}, \frac{1}{2}) \), the reciprocal intercepts are:

\[
\frac{1}{x} = 3, \quad \frac{1}{y} = -\frac{3}{2}, \quad \frac{1}{z} = 2.
\]

Multiplying by 2 to clear the fraction, the Miller indices are \((6 \bar{3} 4)\).

3.50 A cubic plane has the following axial intercepts: \( a = -\frac{1}{2}, \ b = -\frac{1}{2}, \ c = \frac{2}{3} \). What are the Miller indices of this plane?

Given the axial intercepts of \((\text{\(-\frac{1}{2}, \text{\(-\frac{1}{2}, \text{\frac{2}{3}}\)})\} \), the reciprocal intercepts are:

\[
\frac{1}{x} = -2, \quad \frac{1}{y} = -2, \quad \frac{1}{z} = \frac{3}{2}.
\]

Multiplying by 2, the Miller indices are \((\bar{4} \bar{4} 3)\).

3.51 A cubic plane has the following axial intercepts: \( a = 1, \ b = \frac{1}{3}, \ c = -\frac{1}{2} \). What are the Miller indices of this plane?

Given the axial intercepts of \((1, \frac{1}{3}, -\frac{1}{2})\), the reciprocal intercepts are:

\[
\frac{1}{x} = 1, \quad \frac{1}{y} = \frac{3}{2}, \quad \frac{1}{z} = -2.
\]

Multiplying by 2, the Miller indices are \((2 \bar{3} \bar{4})\).

3.52 Determine the Miller indices of the cubic crystal plane that intersects the following position coordinates: \((1, 0, 0); \ (1, \frac{1}{2}, \frac{1}{4}); \ (\frac{1}{2}, \frac{1}{2}, 0)\).

First locate the three position coordinates as shown. Next, connect points \(a\) and \(b\), extending the line to point \(d\) and connect \(a\) to \(c\) and extend to \(e\). Complete the plane by
connecting point \( d \) to \( e \). Using \((1, 1, 0)\) as the plane origin, \(x = -1, \ y = -1\) and \(z = \frac{1}{2}\). The intercept reciprocals are thus \( \frac{1}{x} = -1, \ \frac{1}{y} = -1, \ \frac{1}{z} = 2 \). The Miller indices are \( \overline{1 \ 1 \ 2} \).

3.53 Determine the Miller indices of the cubic crystal plane that intersects the following position coordinates: \((\frac{1}{2}, 0, \frac{1}{2})\); \((0, 0, 1)\); \((1, 1, 1)\).

First locate the three position coordinates as shown. Next, connect points \( a \) and \( b \) and extend the line to point \( d \). Complete the plane by connecting point \( d \) to \( c \) and point \( c \) to \( b \). Using \((1, 0, 1)\) as the plane origin, \(x = -1, \ y = 1\) and \(z = -1\). The intercept reciprocals are thus \( \frac{1}{x} = -1, \ \frac{1}{y} = 1, \ \frac{1}{z} = -1 \). The Miller indices are \( \overline{1 \ 1 \ 1} \).

3.54 Determine the Miller indices of the cubic crystal plane that intersects the following position coordinates: \((1, \frac{1}{2}, 1)\); \((\frac{1}{2}, 0, \frac{3}{4})\); \((1, 0, \frac{1}{2})\).

After locating the three position coordinates, connect points \( b \) and \( c \) and extend the line to point \( d \). Complete the plane by connecting point \( d \) to \( a \) and \( a \) to \( c \). Using \((1, 0, 1)\) as the plane origin, \(x = -1, \ y = \frac{1}{2} \) and \(z = -\frac{1}{2} \). The intercept reciprocals then become \( \frac{1}{x} = -1, \ \frac{1}{y} = 2, \ \frac{1}{z} = -2 \). The Miller indices are \( \overline{1 \ 2 \ 2} \).
3.55 Determine the Miller indices of the cubic crystal plane that intersects the following position coordinates: \((0, 0, \frac{1}{2}); (1, 0, 0); (\frac{1}{2}, \frac{1}{4}, 0)\).

After locating the three position coordinates, connect points \(b\) and \(c\) and extend the line to point \(d\). Complete the plane by connecting point \(d\) to \(a\) and \(a\) to \(b\). Using \((0, 0, 0)\) as the plane origin, \(x = 1, y = \frac{1}{2}\) and \(z = \frac{1}{2}\). The intercept reciprocals are thus \(\frac{1}{x} = 1, \frac{1}{y} = 2, \frac{1}{z} = 2\). The Miller indices are therefore \((1 2 2)\).

3.56 Rodium is FCC and has a lattice constant \(a\) of 0.38044 nm. Calculate the following interplanar spacings:

(a) \(d_{111}\)
(b) \(d_{200}\)
(c) \(d_{220}\)

(a) \(d_{111} = \frac{0.38044 \text{ nm}}{\sqrt{1^2 + 1^2 + 1^2}} = \frac{0.38044 \text{ nm}}{\sqrt{3}} = 0.220 \text{ nm}\)

(b) \(d_{200} = \frac{0.38044 \text{ nm}}{\sqrt{2^2 + 0^2 + 0^2}} = \frac{0.38044 \text{ nm}}{\sqrt{4}} = 0.190 \text{ nm}\)

(c) \(d_{220} = \frac{0.38044 \text{ nm}}{\sqrt{2^2 + 2^2 + 0^2}} = \frac{0.38044 \text{ nm}}{\sqrt{8}} = 0.135 \text{ nm}\)
3.57 Tungsten is BCC and has a lattice constant $a$ of 0.31648 nm. Calculate the following interplanar spacings:
(a) $d_{110}$  
(b) $d_{220}$  
(c) $d_{310}$

(a) $d_{110} = \frac{0.31648 \text{ nm}}{\sqrt{1^2 + 1^2 + 0^2}} = \frac{0.31648 \text{ nm}}{\sqrt{2}} = 0.224 \text{ nm}$

(b) $d_{220} = \frac{0.31648 \text{ nm}}{\sqrt{2^2 + 2^2 + 0^2}} = \frac{0.31648 \text{ nm}}{\sqrt{8}} = 0.112 \text{ nm}$

(c) $d_{310} = \frac{0.31648 \text{ nm}}{\sqrt{3^2 + 1^2 + 0^2}} = \frac{0.31648 \text{ nm}}{\sqrt{10}} = 0.100 \text{ nm}$

3.58 The $d_{310}$ interplanar spacing in a BCC element is 0.1587 nm. (a) What is its lattice constant $a$? (b) What is the atomic radius of the element? (c) What could this element be?

(a) $a = d_{310}\sqrt{h^2 + k^2 + l^2} = (0.1587 \text{ nm})\sqrt{3^2 + 1^2 + 0^2} = 0.502 \text{ nm}$

(b) $R = \frac{\sqrt{3}a}{4} = \frac{\sqrt{3}(0.502 \text{ nm})}{4} = 0.217 \text{ nm}$

(c) The element is barium (Ba).

3.59 The $d_{422}$ interplanar spacing in a FCC metal is 0.083397 nm. (a) What is its lattice constant $a$? (b) What is the atomic radius of the metal? (c) What could this metal be?

(a) $a = d_{422}\sqrt{h^2 + k^2 + l^2} = (0.083397 \text{ nm})\sqrt{4^2 + 2^2 + 2^2} = 0.408 \text{ nm}$

(b) $R = \frac{\sqrt{2}a}{4} = \frac{\sqrt{2}(0.408 \text{ nm})}{4} = 0.144 \text{ nm}$

(c) The element is gold (Au).
3.60 How are crystallographic planes indicated in HCP unit cells?

In HCP unit cells, crystallographic planes are indicated using four indices which correspond to four axes: three basal axes of the unit cell, \(a_1, a_2,\) and \(a_3\), which are separated by 120°; and the vertical \(c\) axis.

3.61 What notation is used to describe HCP crystal planes?

HCP crystal planes are described using the Miller-Bravais indices, \((hkil)\).

3.62 Draw the hexagonal crystal planes whose Miller-Bravais indices are:

(a) \((10\overline{1}1)\)  (d) \((1\overline{2}12)\)  (g) \((\overline{1}2\overline{1}2)\)  (j) \((\overline{1}100)\)

(b) \((01\overline{1}1)\)  (e) \((2\overline{1}\overline{1}1)\)  (h) \((2\overline{2}00)\)  (k) \((\overline{2}111)\)

(c) \((\overline{1}2\overline{1}0)\)  (f) \((1\overline{1}01)\)  (i) \((10\overline{1}2)\)  (l) \((\overline{1}012)\)

The reciprocals of the indices provided give the intercepts for the plane \((a_1, a_2, a_3,\) and \(c)\).

\[
\begin{align*}
\text{(a) } & a_1 = 1, & a_2 &= \infty, & a_3 &= -1, & c &= 1 \\
\text{(d) } & a_1 = 1, & a_2 &= -\frac{1}{2}, & a_3 &= 1, & c &= \frac{1}{2} \\
\text{(b) } & a_1 = \infty, & a_2 &= 1, & a_3 &= -1, & c &= 1 \\
\text{(e) } & a_1 = \frac{1}{2}, & a_2 &= 1, & a_3 &= -1, & c &= 1 \\
\text{(f) } & a_1 = 1, & a_2 &= -1, & a_3 &= \infty, & c &= 1 \\
\end{align*}
\]
3.63 Determine the Miller-Bravais indices of the hexagonal crystal planes in Fig. P3.63.

Miller-Bravais Indices for Planes Shown in Figure P3.63(a)

<table>
<thead>
<tr>
<th>Plane a</th>
<th>Plane b</th>
<th>Plane c</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Planar Intercepts</strong></td>
<td><strong>Reciprocals of Intercepts</strong></td>
<td><strong>Planar Intercepts</strong></td>
</tr>
<tr>
<td>$a_1 = \infty$</td>
<td>$\frac{1}{a_1} = 0$</td>
<td>$a_1 = 1$</td>
</tr>
<tr>
<td>$a_2 = -1$</td>
<td>$\frac{1}{a_2} = -1$</td>
<td>$a_2 = \infty$</td>
</tr>
<tr>
<td>$a_3 = 1$</td>
<td>$\frac{1}{a_3} = 1$</td>
<td>$a_3 = -1$</td>
</tr>
</tbody>
</table>
### Miller-Bravais Indices for the Planes Shown in Figure P3.63(b)

<table>
<thead>
<tr>
<th>Plane a</th>
<th>Planar Intercepts</th>
<th>Planar Intercepts</th>
<th>Planar Intercepts</th>
<th>Planar Intercepts</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( a_1 = \infty )</td>
<td>( \frac{1}{a_1} = 0 )</td>
<td>( a_2 = 1 )</td>
<td>( \frac{1}{a_2} = 1 )</td>
</tr>
<tr>
<td></td>
<td>( a_3 = -1 )</td>
<td>( \frac{1}{a_3} = 1 )</td>
<td>( c = \infty )</td>
<td>( \frac{1}{c} = 0 )</td>
</tr>
<tr>
<td></td>
<td>The Miller indices of plane ( a ) are (0 1 1 0).</td>
<td>The Miller indices of plane ( b ) are (1 1 0 1).</td>
<td>The Miller indices of plane ( c ) are (1 1 0 1).</td>
<td></td>
</tr>
</tbody>
</table>

3.64 Determine the Miller-Bravais direction indices of the \(-a_1\), \(-a_2\) and \(-a_3\) directions.

The Miller-Bravais direction indices corresponding to the \(-a_1\), \(-a_2\) and \(-a_3\) directions are respectively, \([\bar{1} 0 0 0]\), \([0 \bar{1} 0 0]\), and \([0 0 \bar{1} 0]\).

3.65 Determine the Miller-Bravais direction indices of the vectors originating at the center of the lower basal plane and ending at the end points of the upper basal plane as indicated in Fig. 3.18(d).

\([\bar{1} 1 2 1], [\bar{2} 1 1 1], [\bar{1} 2 \bar{1} 1], [1 1 \bar{2} 1], [1 2 \bar{1} 1], [1 \bar{2} \bar{1} 1]\)
3.66 Determine the Miller-Bravais direction indices of the basal plane of the vectors originating at the center of the lower basal plane and exiting at the midpoints between the principal planar axes.

\[ \{3\,0\,3\,4\} , \{3\,3\,0\,4\} , \{0\,3\,3\,4\} , \{3\,0\,3\,4\} , \{3\,3\,0\,4\} , \{0\,3\,3\,4\} \]

3.67 Determine the Miller-Bravais direction indices of the directions indicated in Fig. P3.67.

For Fig. P3.67(a), the Miller-Bravais direction indices indicated are \[ \{2\,1\,1\,1\} \] and \[ \{1\,1\,\bar{2}\,1\} \]. Those associated with Fig. P3.67(b) are \[ \{\bar{1}\,1\,0\,1\} \] and \[ \{1\,0\,1\,1\} \].

3.68 What is the difference in the stacking arrangement of close-packed planes in (a) the HCP crystal structure and (b) the FCC crystal structure?

Although the FCC and HCP are both close-packed lattices with APF = 0.74, the structures differ in the three dimensional stacking of their planes:

(a) the stacking order of HCP planes is ABAB… ;
(b) the FCC planes have an ABCABC… stacking sequence.

3.69 What are the densest-packed planes in (a) the FCC structure and (b) the HCP structure?

(a) The most densely packed planes of the FCC lattice are the \{1\,1\,1\} planes.
(b) The most densely packed planes of the HCP structure are the \{0\,0\,0\,1\} planes.

3.70 What are the closest-packed directions in (a) the FCC structure and (b) the HCP structure?

(a) The closest-packed directions in the FCC lattice are the \{1\,\bar{1}\,0\} directions.
(b) The closest-packed directions in the HCP lattice are the \{1\,1\,\bar{2}\,0\} directions.
3.71 The lattice constant for BCC tantalum at 20ºC is 0.33026 nm and its density is 16.6 g/cm³. Calculate a value for its atomic mass.

The atomic mass can be assessed based upon the mass of tantalum in a unit BCC cell:

\[
\text{mass/unit cell} = \rho_o (\text{volume/unit cell}) = \rho_o a^3
\]

\[
= (16.6 \text{ g/cm}^3)(10^6 \text{ cm}^3/\text{m}^3)(0.33026 \times 10^{-9} \text{ m})^3
\]

\[
= 5.98 \times 10^{-22} \text{ g/u.c.}
\]

Since there are two atoms in a BCC unit cell, the atomic mass is:

\[
\text{Atomic mass} = \frac{(5.98 \times 10^{-22} \text{ g/unit cell})(6.023 \times 10^{23} \text{ atoms/mol})}{2 \text{ atoms/unit cell}}
\]

\[
= 180.09 \text{ g/mol}
\]

3.72 Calculate a value for the density of FCC platinum in grams per cubic centimeter from its lattice constant \(a\) of 0.39239 nm and its atomic mass of 195.09 g/mol.

First calculate the mass per unit cell based on the atomic mass and the number of atoms per unit cell of the FCC structure,

\[
\text{mass/unit cell} = \frac{(4 \text{ atoms/unit cell})(195.09 \text{ g/mol})}{6.023 \times 10^{23} \text{ atoms/mol}} = 1.296 \times 10^{-21} \text{ g/unit cell}
\]

The density is then found as,

\[
\rho_o = \frac{\text{mass/unit cell}}{\text{volume/unit cell}} = \frac{1.296 \times 10^{-21} \text{ g/unit cell}}{(0.39239 \times 10^{-9} \text{ m})^3/\text{unit cell}}
\]

\[
= 21,445,113 \text{ g/m}^3 \left(\frac{\text{m}}{100 \text{ cm}}\right)^3 = 21.45 \text{ g/cm}^3
\]

3.73 Calculate the planar atomic density in atoms per square millimeter for the following crystal planes in BCC chromium, which has a lattice constant of 0.28846 nm: (a) (100), (b) (110), (c) (111).
To calculate the density, the planar area and the number of atoms contained in that area must first be determined.

(a) The area intersected by the (1 0 0) plane inside the cubic unit cell is \(a^2\). The number of atoms contained is: (4 corners) \(\times (\frac{1}{4} \text{ atom per corner}) = 1 \text{ atom}\). The density is,

\[
\rho_p = \frac{\text{equiv. no. of atoms whose centers are intersected by selected area}}{\text{selected area}} = \frac{1 \text{ atom}}{(0.28846 \times 10^{-9} \text{ m})^2} = (1.202 \times 10^{19} \text{ atoms/m}^2) \left(\frac{\text{m}}{1000 \text{ mm}}\right)^2
\]

\[
= 1.202 \times 10^{13} \text{ atoms/mm}^2
\]

(b) For the more densely packed (1 1 0) plane, there are:

1 atom at center + (4 corners) \(\times (\frac{1}{4} \text{ atom per corner}) = 2 \text{ atoms}\)

And the area is given as \((\sqrt{2}a)(a) = \sqrt{2}a^2\). The density is thus,

\[
\rho_p = \frac{2 \text{ atoms}}{\sqrt{2}(0.28846 \times 10^{-9} \text{ m})^2} = (1.699 \times 10^{19} \text{ atoms/m}^2) (10^{-6} \text{ m}^2/\text{mm}^2)
\]

\[
= 1.699 \times 10^{13} \text{ atoms/mm}^2
\]

(c) The triangular (1 1 1) plane contains: (3 corners) \(\times (\frac{1}{6} \text{ atom per corner}) = \frac{1}{2} \text{ atom}\).

The area is equal to:

\[
\frac{1}{2} bh = \frac{1}{2} (\sqrt{2}a) \left(\frac{\sqrt{3}}{2} a\right) = \frac{\sqrt{6}}{4} a^2
\]

The density is thus,

\[
\rho_p = \frac{\frac{1}{2} \text{ atom}}{\frac{\sqrt{6}}{4} (0.28846 \times 10^{-9} \text{ m})^2} = (9.813 \times 10^{18} \text{ atoms/m}^2)(10^{-6} \text{ m}^2/\text{mm}^2)
\]

\[
= 9.813 \times 10^{12} \text{ atoms/mm}^2
\]

3.74 Calculate the planar atomic density in atoms per square millimeter for the following crystal planes in FCC gold, which has a lattice constant of 0.40788 nm: (a) (100), (b) (110), (c) (111).
(a) The area intersected by the (1 0 0) plane and the FCC unit cell is \( a^2 \) while the number of atoms contained is:

\[
1 \text{ atom at center} + (4 \text{ corners}) \times (\frac{1}{4} \text{ atom per corner}) = 2 \text{ atoms}
\]

The density is therefore,

\[
\rho_p = \frac{\text{equiv. no. of atoms whose centers are intersected by selected area}}{\text{selected area}} = \frac{2 \text{ atoms}}{(0.40788 \times 10^{-9} \text{ m})^2} = (1.202 \times 10^{19} \text{atoms/m}^2) \left( \frac{\text{m}}{1000 \text{ mm}} \right)^2
\]

\[= 1.20 \times 10^{13} \text{ atoms/mm}^2\]

(b) For the more densely packed (1 1 0) plane, there are:

\[
(2 \text{ face atoms}) \times (\frac{1}{2} \text{ atom}) + (4 \text{ corners}) \times (\frac{1}{4} \text{ atom per corner}) = 2 \text{ atoms}
\]

And the area is given as \((\sqrt{2}a)(a) = \sqrt{2}a^2\). The density is thus,

\[
\rho_p = \frac{2 \text{ atoms}}{\sqrt{2}(0.40788 \times 10^{-9} \text{ m})^2} = (8.501 \times 10^{18} \text{atoms/m}^2)(10^{-6} \text{ m}^2/\text{mm}^2)
\]

\[= 8.50 \times 10^{12} \text{ atoms/mm}^2\]

(c) The triangular (1 1 1) plane contains:

\[
(3 \text{ face atoms} \times \frac{1}{3} \text{ atom}) + (3 \text{ corners}) \times (\frac{1}{6} \text{ atom per corner}) = 2 \text{ atoms}
\]

The area is equal to:

\[
\frac{1}{2} bh = \frac{1}{2} (\sqrt{2}a) \left( \frac{\sqrt{3}}{2} a \right) = \frac{\sqrt{6}}{4} a^2.
\]

The density is therefore,

\[
\rho_p = \frac{2 \text{ atoms}}{\frac{\sqrt{6}}{4} (0.40788 \times 10^{-9} \text{ m})^2} = (1.963 \times 10^{19} \text{atoms/m}^2)(10^{-6} \text{ m}^2/\text{mm}^2)
\]

\[= 1.963 \times 10^{13} \text{ atoms/mm}^2\]

3.75 Calculate the planar atomic density in atoms per square millimeter for the (0001) plane in HCP beryllium which has a constant \( a = 0.22856 \text{ nm} \) and a \( c \) constant of 0.35832 \text{ nm}.

The area intersected by the (0 0 0 1) plane and the HCP unit cell is simply the basal area, shown in the sketch to the right:
Selected Area = (6 triangles) × (equilateral triangle area) = 6 \left( \frac{1}{2} a \right) \left( \frac{\sqrt{3}}{2} a \right) = \frac{3\sqrt{3}}{2} a^2

While the number of atoms contained is:

1 atom at center + (6 corners) × (1/3 atom per corner) = 3 atoms

The density is therefore,

\[ \rho_p = \frac{\text{equiv. no. of atoms whose centers are intersected by selected area}}{\text{selected area}} \]

\[ = \frac{3 \text{ atoms}}{\frac{3\sqrt{3}}{2} \left(0.22856 \times 10^{-9} \text{ m}\right)^2} = \left(2.201 \times 10^{19} \text{ atoms/m}^2\right) \left(\frac{\text{m}}{1000 \text{ mm}}\right)^2 \]

\[ = 2.21 \times 10^{13} \text{ atoms/mm}^2 \]

3.76 Calculate the linear atomic density in atoms per millimeter for the following directions in BCC vanadium, which has a lattice constant of 0.3039 nm:
(a) [100], (b) [110], (c) [111].

In general, the linear atomic density is derived from:

\[ \rho_l = \frac{\text{no. of atomic diam. intersected by selected length of direction line}}{\text{selected length of line}} \]

(a) For the [100] direction of BCC vanadium,

\[ \rho_l = \frac{\text{no. atom dia.}}{a} = \frac{1 \text{ atom}}{(0.3039 \text{ nm})(10^{-9} \text{ m/nm})(10^3 \text{ mm/m})} = 3.29 \times 10^6 \text{ mm} \]

(b) For the [110] direction of BCC vanadium,
\[
\rho_i = \frac{\text{no. atom dia.}}{\sqrt{2}a} = \frac{1 \text{ atom}}{\sqrt{2}(0.3039 \text{ nm})(10^{-6} \text{ mm/nm})} = 2.33 \times 10^6 \text{ mm}
\]

(c) For the [111] direction of BCC vanadium,

\[
\rho_i = \frac{\text{no. atom dia.}}{\sqrt{3}a} = \frac{2 \text{ atoms}}{\sqrt{3}(0.3039 \text{ nm})(10^{-6} \text{ mm/nm})} = 3.80 \times 10^6 \text{ mm}
\]

3.77 Calculate the linear atomic density in atoms per millimeter for the following directions in FCC iridium, which has a lattice constant of 0.38389 nm:

(a) [100], (b) [110], (c) [111].

In general, the linear atomic density is derived from:

\[
\rho_i = \frac{\text{no. of atomic diam. intersected by selected length of direction line}}{\text{selected length of line}}
\]

(a) For the [100] direction of FCC iridium,

\[
\rho_i = \frac{\text{no. atom dia.}}{a} = \frac{1 \text{ atom}}{(0.38389 \text{ nm})(10^{-6} \text{ mm/nm})} = 2.60 \times 10^6 \text{ mm}
\]

(b) For the [110] direction of FCC iridium,

\[
\rho_i = \frac{\text{no. atom dia.}}{\sqrt{2}a} = \frac{2 \text{ atoms}}{\sqrt{2}(0.38389 \text{ nm})(10^{-6} \text{ mm/nm})} = 3.68 \times 10^6 \text{ mm}
\]

(c) For the [111] direction of FCC iridium,

\[
\rho_i = \frac{\text{no. atom dia.}}{\sqrt{3}a} = \frac{1 \text{ atom}}{\sqrt{3}(0.38389 \text{ nm})(10^{-6} \text{ mm/nm})} = 1.50 \times 10^6 \text{ mm}
\]
What is polymorphism with respect to metals?

A metal is considered polymorphic if it can exist in more than one crystalline form under different conditions of temperature and pressure.

Titanium goes through a polymorphic change from BCC to HCP crystal structure upon cooling through 882°C. Calculate the percentage change in volume when the crystal structure changes from BCC to HCP. The lattice constant \( a \) of the BCC unit cell at 882°C is 0.332 nm and the HCP unit cell has \( a = 0.2950 \) nm and \( c = 0.4683 \) nm.

To determine the volume change, the individual volumes per atom for the BCC and HCP structures must be calculated:

\[
V_{\text{BCC}} = \frac{a^3}{2 \text{ atoms/unit cell}} = \frac{(0.332 \text{ nm})^3}{2 \text{ atoms}} = 0.0183 \text{ nm}^3/\text{atom}
\]

\[
V_{\text{HCP}} = \frac{(3a^2c)(\sin 60^\circ)}{6 \text{ atoms/unit cell}} = \frac{(3)(0.2950 \text{ nm})^2(0.4683 \text{ nm})(\sin 60^\circ)}{6 \text{ atoms}} = 0.01765 \text{ nm}^3/\text{atom}
\]

Thus the change in volume due to titanium’s allotropic transformation is,

\[
\% \text{ Volume change} = \frac{V_{\text{HCP}} - V_{\text{BCC}}}{V_{\text{BCC}}} (100\%) = \frac{0.01765 \text{ nm}^3/\text{atom} - 0.0183 \text{ nm}^3/\text{atom}}{0.0183 \text{ nm}^3/\text{atom}} (100\%) = -3.55\%
\]

Pure iron goes through a polymorphic change from BCC to FCC upon heating through 912°C. Calculate the volume change associated with the change in crystal structure from BCC to FCC if at 912°C the BCC unit cell has a lattice constant \( a = 0.293 \) nm and the FCC unit cell \( a = 0.363 \).

First determine the individual volumes per atom for the iron BCC and FCC crystal structures:

\[
V_{\text{BCC}} = \frac{a^3}{2 \text{ atoms/unit cell}} = \frac{(0.293 \text{ nm})^3}{2 \text{ atoms}} = 0.01258 \text{ nm}^3/\text{atom}
\]

\[
V_{\text{FCC}} = \frac{a^3}{4 \text{ atoms/unit cell}} = \frac{(0.363 \text{ nm})^3}{4 \text{ atoms}} = 0.01196 \text{ nm}^3/\text{atom}
\]

Thus the change in volume due to iron’s allotropic transformation is,
% Volume change = \frac{V_{FCC} - V_{BCC}}{V_{BCC}}(100\%) = \frac{0.01196 \text{ nm}^3/\text{atom} - 0.01258 \text{ nm}^3/\text{atom}}{0.01258 \text{ nm}^3/\text{atom}}(100\%) = -4.94\%

3.81 What are x-rays, and how are they produced?

X-rays are electromagnetic radiation having wavelengths in the range of approximately 0.05 nm to 0.25 nm. These waves are produced when accelerated electrons strike a target metal.

3.82 Draw a schematic diagram of an x-ray tube used for x-ray diffraction, and indicate on it the path of the electrons and x-rays.

See Figure 3.25 of textbook.

3.83 What is the characteristic x-ray radiation? What is its origin?

Characteristic radiation is an intense form of x-ray radiation which occurs at specific wavelengths for a particular element. The $K_\alpha$ radiation, the most intense characteristic radiation emitted, is caused by excited electrons dropping from the second atomic shell (n = 2) to the first shell (n = 1). The next most intense radiation, $K_\beta$, is caused by excited electrons dropping from the third atomic shell (n = 3) to the first shell (n = 1).

3.84 Distinguish between destructive interference and constructive interference of reflected x-ray beams through crystals.

Destructive interference occurs when the wave patterns of an x-ray beam, reflected from a crystal, are out of phase. Conversely, when the wave patterns leaving a crystal plane are in phase, constructive interference occurs and the beam is reinforced.

3.85 Derive Bragg’s law by using the simple case of incident x-ray beams being diffracted by parallel planes in a crystal.

Referring to Fig. 3.28 (c), for these rays to be in phase, ray 2 must travel an additional distance of $MP + PN$. This extra length must be an integral number of wavelengths, $\lambda$.

\[ n\lambda = MP + PN \text{ where } n = 1, 2, 3... \]

Moreover, the $MP$ and $PN$ distances must equal $d_{hkl} \sin \theta$, where $d_{hkl}$ is the crystal interplanar spacing required for constructive interference.

\[ MP = d_{hkl} \sin \theta \text{ and } PN = d_{hkl} \sin \theta \]

Substituting,
\[ n\lambda = 2d_{hkl} \sin \theta \quad \text{Bragg's Law} \]

3.86 A sample of BCC metal was placed in an x-ray diffractometer using x-rays with a wavelength of \( \lambda = 0.1541 \, \text{nm} \). Diffraction from the \{221\} planes was obtained at \( 2\theta = 88.838^\circ \). Calculate a value for the lattice constant \( a \) for this BCC elemental metal (Assume first-order diffraction, \( n = 1 \)).

The interplanar distance is,

\[ d_{221} = \frac{\lambda}{2 \sin \theta} = \frac{0.1541 \, \text{nm}}{2 \sin(44.419^\circ)} = 0.1101 \, \text{nm} \]

The lattice constant, \( a \), is then,

\[ a = d_{hkl} \sqrt{h^2 + k^2 + l^2} = (0.1101 \, \text{nm}) \sqrt{2^2 + 2^2 + 1^2} = 0.3303 \, \text{nm} \]

3.87 X-rays of an unknown wavelength are diffracted by a gold sample. The \( 2\theta \) angle was 64.582\(^\circ\) for the \{220\} planes. What is the wavelength of the x-rays used? (The lattice constant of gold is 0.40788 nm. Assume first-order diffraction, \( n = 1 \)).

The interplanar distance is,

\[ d_{220} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{0.40788 \, \text{nm}}{\sqrt{2^2 + 2^2 + 0^2}} = 0.1442 \, \text{nm} \]

The lattice constant, \( a \), is then,

\[ \lambda = 2d_{221} \sin \theta = 2(0.1442 \, \text{nm}) \sin(32.291^\circ) = 0.154 \, \text{nm} \]

3.88 An x-ray diffractometer recorder chart for an element which has either the BCC or the FCC crystal structure showed diffraction peaks at the following \( 2\theta \) angles: 41.069\(^\circ\), 47.782\(^\circ\), 69.879\(^\circ\), and 84.396\(^\circ\). (The wavelength of the incoming radiation was 0.15405 nm.)

(a) Determine the crystal structure of the element.
(b) Determine the lattice constant of the element.
(c) Identify the element.

(a) Comparing the \( \sin^2 \theta \) term for the first two angles:

<table>
<thead>
<tr>
<th>( 2\theta )</th>
<th>( \theta )</th>
<th>( \sin \theta )</th>
<th>( \sin^2 \theta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>41.069(^\circ)</td>
<td>20.535(^\circ)</td>
<td>0.35077</td>
<td>0.12304</td>
</tr>
<tr>
<td>47.782(^\circ)</td>
<td>23.891(^\circ)</td>
<td>0.40499</td>
<td>0.16402</td>
</tr>
</tbody>
</table>
\[
\frac{\sin^2 \theta_1}{\sin^2 \theta_2} = \frac{0.12304}{0.16402} = 0.75 \Rightarrow \text{FCC}
\]

(b) The lattice constant also depends upon the first \(\sin^2 \theta\) term, as well as, the Miller indices of the first set of FCC principal diffracting planes, \(\{111\}\).

\[
a = \frac{\lambda}{2} \sqrt{\frac{h^2 + k^2 + l^2}{\sin^2 \theta_1}} = \frac{0.15405 \text{ nm}}{2} \sqrt{\frac{1^2 + 1^2 + 1^2}{0.12304}} = 0.38034 \text{ nm}
\]

(c) From Appendix I, the FCC metal whose lattice constant is closest to 0.38034 nm is **rhodium (Rh)** which has a lattice constant of 0.38044 nm.

3.89 An x-ray diffractometer recorder chart for an element which has either the BCC or the FCC crystal structure showed diffraction peaks at the following 20 angles: 38.60°, 55.71°, 69.70°, 82.55°, 95.00°, and 107.67°. (The wavelength \(\lambda\) of the incoming radiation was 0.15405 nm.)

(a) Determine the crystal structure of the element.

(b) Determine the lattice constant of the element.

(c) Identify the element.

(a) Comparing the \(\sin^2 \theta\) term for the first two angles:

<table>
<thead>
<tr>
<th>(2\theta)</th>
<th>(\theta)</th>
<th>(\sin \theta)</th>
<th>(\sin^2 \theta)</th>
</tr>
</thead>
<tbody>
<tr>
<td>38.60°</td>
<td>19.30°</td>
<td>0.33051</td>
<td>0.10924</td>
</tr>
<tr>
<td>55.71°</td>
<td>27.855°</td>
<td>0.46724</td>
<td>0.21831</td>
</tr>
</tbody>
</table>

\[
\frac{\sin^2 \theta_1}{\sin^2 \theta_2} = \frac{0.10924}{0.21831} = 0.50 \Rightarrow \text{BCC}
\]

(b) The lattice constant also depends upon the first \(\sin^2 \theta\) term, as well as, the Miller indices of the first set of BCC principal diffracting planes \(\{110\}\).

\[
a = \frac{\lambda}{2} \sqrt{\frac{h^2 + k^2 + l^2}{\sin^2 \theta_1}} = \frac{0.15405 \text{ nm}}{2} \sqrt{\frac{1^2 + 1^2 + 0^2}{0.10924}} = 0.3296 \text{ nm}
\]

(c) From Appendix I, the BCC metal whose lattice constant is closest to 0.3296 nm is **niobium (Nb)** which has a lattice constant of 0.33007 nm.
An x-ray diffractometer recorder chart for an element which has either the BCC or the FCC crystal structure showed diffraction peaks at the following 2θ angles: 36.191°, 51.974°, 64.982°, and 76.663°. (The wavelength λ of the incoming radiation was 0.15405 nm.)

(a) Determine the crystal structure of the element.
(b) Determine the lattice constant of the element.
(c) Identify the element.

(a) Comparing the \( \sin^2 \theta \) term for the first two angles:

<table>
<thead>
<tr>
<th>2θ</th>
<th>θ</th>
<th>( \sin \theta )</th>
<th>( \sin^2 \theta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>36.191°</td>
<td>18.096°</td>
<td>0.31060</td>
<td>0.09647</td>
</tr>
<tr>
<td>51.974°</td>
<td>25.987°</td>
<td>0.43817</td>
<td>0.19199</td>
</tr>
</tbody>
</table>

\[ \frac{\sin^2 \theta_1}{\sin^2 \theta_2} = \frac{0.09647}{0.19199} = 0.50 \implies \text{BCC} \]

(b) The lattice constant also depends upon the first \( \sin^2 \theta \) term, as well as, the Miller indices of the first set of BCC principal diffracting planes, \{110\}.

\[
a = \frac{\lambda}{2} \sqrt{\frac{h^2 + k^2 + l^2}{\sin^2 \theta_1}} = \frac{0.15405 \text{ nm}}{2} \sqrt{\frac{1^2 + 1^2 + 0^2}{0.09647}} = 0.35071 \text{ nm}
\]

(c) From Appendix I, the BCC metal whose lattice constant is closest to 0.35071 nm is lithium (Li) which has a lattice constant of 0.35092 nm.

An x-ray diffractometer recorder chart for an element which has either the BCC or the FCC crystal structure showed diffraction peaks at the following 2θ angles: 40.663°, 47.314°, 69.144°, and 83.448°. (The wavelength λ of the incoming radiation was 0.15405 nm.)

(a) Determine the crystal structure of the element.
(b) Determine the lattice constant of the element.
(c) Identify the element.

(a) Comparing the \( \sin^2 \theta \) term for the first two angles:

<table>
<thead>
<tr>
<th>2θ</th>
<th>θ</th>
<th>( \sin \theta )</th>
<th>( \sin^2 \theta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>40.663°</td>
<td>20.3315°</td>
<td>0.34745</td>
<td>0.12072</td>
</tr>
<tr>
<td>47.314°</td>
<td>23.657°</td>
<td>0.40126</td>
<td>0.16101</td>
</tr>
</tbody>
</table>
\[
\frac{\sin^2 \theta_1}{\sin^2 \theta_2} = \frac{0.12072}{0.16101} = 0.75 \Rightarrow \text{FCC}
\]

(b) The lattice constant also depends upon the first \(\sin^2 \theta\) term, as well as, the Miller indices of the first set of FCC principal diffracting planes, \{111\}.

\[
a = \frac{\lambda}{2} \sqrt{\frac{h^2 + k^2 + l^2}{\sin^2 \theta_1}} = \frac{0.15405 \text{ nm}}{2} \sqrt{\frac{1^2 + 1^2 + 1^2}{0.12072}} = 0.38397 \text{ nm}
\]

(c) From Appendix I, the FCC metal whose lattice constant is closest to 0.38397 nm is \textbf{iridium (Ir)} which has a lattice constant of 0.38389 nm.