1. Why is it essential to study materials engineering and modern materials need?

2. Discuss and explain materials engineering classification.
   Answer: discuss and explain regarding metals, ceramics and polymers.

3. Cite the difference between atomic mass and atomic weight.
   Answer: 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.

4. (a) How many grams are there in one amu of a material?
   (b) Mole, in the context of our textbook, is taken in units of gram-mole. On this basis, how many atoms are there in a gram-mole of a substance?
   Answer:
   (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
   \[
   \# \text{g/amu} = \left( \frac{1 \text{ mol}}{6.022 \times 10^{23} \text{ atoms}} \right) \left( \frac{1 \text{ g/mol}}{1 \text{ amu/atom}} \right)
   \]
   \[
   = 1.66 \times 10^{-24} \text{ g/amu}
   \]
   (b) There are $6.022 \times 10^{23}$ atoms/g-mol in a substance.

5. (a) Relative to electrons and electron states, what does each of the four quantum numbers specify?
   (b) Cite two important quantum mechanical concepts associated with the Bohr model of the atom.
   (c) Cite two important additional refinements that resulted from the Wave-mechanical atomic model.
   Answers:
   (a) n quantum number designates the electron shell.
   l quantum number designates the electron subshell.
   ml quantum number designates the no. of electron states in each electron subshell.
   ms quantum number designates the spin moment on each electron.
(b) Two important quantum-mechanical concepts associated with the Bohr model of the atom are (1) that electrons are particles moving in discrete orbitals, and (2) electron energy is quantized into shells.

(c) Two important refinements resulting from the wave-mechanical atomic model are (1) that electron position is described in terms of a probability distribution, and (2) electron energy is quantized into both shells and subshells—each electron is characterized by four quantum numbers.

6. Give the electron configurations for the following ions: Fe$^{2+}$, Al$^{3+}$, Cu$^{+}$, Ba$^{2+}$, Br$^{-}$, O$^{2-}$, Fe$^{3+}$ and S$^{2-}$.

Answer:

Fe$^{2+}$: From Table 2.2, the electron configuration for an atom of iron is 1s$^2$2s$^2$2p$^6$3s$^2$3p$^6$3d$^5$. In order to become an ion with a plus two charge, it must lose two electrons—in this case the two 4s. Thus, the electron configuration for an Fe$^{2+}$ ion is 1s$^2$2s$^2$2p$^6$3s$^2$3p$^6$3d$^9$.

Al$^{3+}$: From Table 2.2, the electron configuration for an atom of aluminum is 1s$^2$2s$^2$2p$^6$3s$^2$3p$^2$. In order to become an ion with a plus three charge, it must lose three electrons—in this case two 3s and the one 3p. Thus, the electron configuration for an Al$^{3+}$ ion is 1s$^2$2s$^2$2p$^6$.

Cu$^{+}$: From Table 2.2, the electron configuration for an atom of copper is 1s$^2$2s$^2$2p$^6$3s$^2$3p$^6$3d$^{10}$4s$^1$. In order to become an ion with a plus one charge, it must lose one electron—in this case the 4s. Thus, the electron configuration for a Cu$^{+}$ ion is 1s$^2$2s$^2$2p$^6$3s$^2$3p$^6$3d$^{10}$.

Ba$^{2+}$: The atomic number for barium is 56 (Figure 2.6), and inasmuch as it is not a transition element the electron configuration for one of its atoms is 1s$^2$2s$^2$2p$^6$3s$^2$3p$^6$3d$^{10}$4s$^2$4p$^6$4d$^{10}$5s$^2$5p$^6$. In order to become an ion with a plus two charge, it must lose two electrons—in this case the two 6s. Thus, the electron configuration for a Ba$^{2+}$ ion is 1s$^2$2s$^2$2p$^6$3s$^2$3p$^6$3d$^{10}$4s$^2$4p$^6$.

Br$^{-}$: From Table 2.2, the electron configuration for an atom of bromine is 1s$^2$2s$^2$2p$^6$3s$^2$3p$^6$3d$^{10}$4s$^2$4p$^5$. In order to become an ion with a minus one charge, it must acquire one electron—in this case another 4p. Thus, the electron configuration for a Br$^{-}$ ion is 1s$^2$2s$^2$2p$^6$3s$^2$3p$^6$3d$^{10}$4s$^2$4p$^6$.

O$^{2-}$: From Table 2.2, the electron configuration for an atom of oxygen is 1s$^2$2s$^2$2p$^4$. In order to become an ion with a minus two charge, it must acquire two electrons—in this case another two 2p. Thus, the electron configuration for an O$^{2-}$ ion is 1s$^2$2s$^2$2p$^6$.

Fe$^{3+}$: From Table 2.2, the electron configuration for an atom of iron is 1s$^2$2s$^2$2p$^6$3s$^2$3p$^6$3d$^5$. In order to become an ion with a plus three charge, it must lose three electrons—in this case the two 4s and one 3d. Thus, the electron configuration for an Fe$^{3+}$ ion is 1s$^2$2s$^2$2p$^6$3s$^2$3p$^6$3d$^8$.

S$^{2-}$: From Table 2.2, the electron configuration for an atom of sulphur is 1s$^2$2s$^2$2p$^6$3s$^2$3p$^4$. In order to become an ion with a minus two charge, it must acquire two electrons—in this case another two 3p. Thus, the electron configuration for an S$^{2-}$ ion is 1s$^2$2s$^2$2p$^6$3s$^2$3p$^6$.

7. Without consulting Figure 2.6 or Table 2.2, determine whether each of the electron configurations given below is an inert gas, a halogen, an alkali metal, an alkaline earth metal, or a transition metal. Justify your choices.

(a) 1s$^2$2s$^2$2p$^6$3s$^2$3p$^6$3d$^7$4s$^2$
(b) 1s²2s²2p⁶3s²3p⁶
(c) 1s²2s²2p⁵
(d) 1s²2s²2p⁶3s²
(e) 1s²2s²2p⁶3s²3p⁶3d²4s²
(f) 1s²2s²2p⁶3s²3p⁶4s¹

Answer:

(a) The 1s²2s²2p⁶3s²3p⁶3d²4s² electron configuration is that of a transition metal because of an incomplete d subshell.
(b) The 1s²2s²2p⁶3s²3p⁶ electron configuration is that of an inert gas because of filled 3s and 3p subshells.
(c) The 1s²2s²2p⁵ electron configuration is that of a halogen because it is one electron deficient from having a filled L shell.
(d) The 1s²2s²2p⁶3s² electron configuration is that of an alkaline earth metal because of two s electrons.
(e) The 1s²2s²2p⁶3s²3p⁶3d²4s² electron configuration is that of a transition metal because of an incomplete d subshell.
(f) The 1s²2s²2p⁶3s²3p⁶4s¹ electron configuration is that of an alkali metal because of a single s electron.

8. What is the difference between atomic structure and crystal structure?

Answer:

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.

Crystal structure pertains to the arrangement of atoms in the crystalline solid material.
9. Show for the body-centered cubic crystal structure that the unit cell edge length $a$ and the atomic radius $R$ are related through $a = 4R/3^{1/2}$.

Answer:

Consider the BCC unit cell shown below.

![BCC unit cell diagram]

Using the triangle $NOP$

$$(OP)^2 = a^2 + a^2 - 2a^2$$

And then for triangle $NPO$,

$$(NO)^2 = (OF)^2 + (NP)^2$$

But $NO = 4R$, $R$ being the atomic radius. Also, $OF = a$. Therefore,

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

or

$$a = \frac{4R}{\sqrt{3}}$$
10. Show that the atomic packing factor for BCC is 0.68.

Answer:

The atomic packing factor is defined as the ratio of sphere volume to the total unit cell volume, or

\[ \text{APF} = \frac{V_s}{V_C} \]

Since there are two spheres associated with each unit cell for BCC

\[ V_s = 2 (\text{sphere volume}) = 2 \left( \frac{4\pi R^3}{3} \right) = \frac{8\pi R^3}{3} \]

Also, the unit cell has cubic symmetry, that is \( V_C = a^3 \). But \( a \) depends on \( R \) according to Equation 3.3, and

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

Thus,

\[ \text{APF} = \frac{V_s}{V_C} = \frac{\frac{8\pi R^3}{3}}{\frac{64R^3}{3\sqrt{3}}} = 0.68 \]
11. Iron has a BCC crystal structure, an atomic radius of 0.124 nm, and an atomic weight of 55.85 g/mol. Compute and compare its theoretical density with the experimental value found in the front section of the textbook.

Answer:

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

\[ \rho = \frac{n_\text{atoms}}{V_c N_A} \]

For BCC, \( n = 2 \) atoms/unit cell, and

\[ V_c = \left( \frac{4R}{\sqrt{3}} \right)^3 \]

Thus,

\[ \rho = \frac{n_\text{atoms}}{\left( \frac{4R}{\sqrt{3}} \right)^3 N_A} \]

\[ = \frac{(2 \text{ atoms/unit cell})(55.85 \text{ g/mol})}{\left[ (4)(0.124 \times 10^{-7} \text{ cm})/\sqrt{3} \right]/(\text{unit cell})(6.022 \times 10^{23} \text{ atoms/mol})} \]

\[ = 7.90 \text{ g/cm}^3 \]

The value given inside the front cover is 7.87 g/cm³.
12. Calculate the radius of a vanadium atom, given that V has a BCC crystal structure, a density of 5.96 g/cm³, and an atomic weight of 50.9 g/mol.

Answer:

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

\[
V_C = \left( \frac{4R^3}{3\sqrt{2}} \right) = \frac{64R^3}{3\sqrt{2}}
\]

Since, from Equation 3.5

\[
\rho = \frac{nA_s}{V_CN_A}
\]

\[
= \frac{nA_s}{\left( \frac{64R^3}{3\sqrt{2}} \right)N_A}
\]

and solving for \( R \) the previous equation

\[
R = \left( \frac{3\sqrt{2}nA_s}{64\rho N_A} \right)^{1/3}
\]

and incorporating values of parameters given in the problem statement

\[
R = \left( \frac{(2\sqrt{2})(2 \text{ atoms/unit cell}) (50.9 \text{ g/mol})}{(64)(5.96 \text{ g/cm}^3)(6.022 \times 10^{23} \text{ atoms/mol})} \right)^{1/3}
\]

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

13. Determine the indices for the directions shown in the following cubic unit cell.

Answer:
Direction A is a $[\overline{4}30]$ 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

$$
\begin{array}{ccc}
\bar{X} & \bar{Y} & \bar{Z} \\
\frac{-2a}{3} & \frac{b}{2} & 0c \\
\frac{-2}{3} & \frac{1}{2} & 0 \\
\end{array}
$$

Projections in terms of $a$, $b$, and $c$

Reduction to integers

Enclosure $[\overline{4}30]$

Direction B is a $[\overline{2}32]$ 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

$$
\begin{array}{ccc}
\bar{X} & \bar{Y} & \bar{Z} \\
\frac{2a}{3} & -\frac{b}{2} & \frac{2c}{3} \\
\frac{2}{3} & -1 & \frac{2}{3} \\
\end{array}
$$

Projections in terms of $a$, $b$, and $c$

Reduction to integers

Enclosure $[\overline{2}32]$

Direction C is a $[\overline{1}33]$ 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

$$
\begin{array}{ccc}
\bar{X} & \bar{Y} & \bar{Z} \\
\frac{a}{3} & -\frac{b}{2} & -c \\
\frac{1}{3} & -1 & -1 \\
\end{array}
$$

Projections in terms of $a$, $b$, and $c$

Reduction to integers

Enclosure $[\overline{1}33]$

Direction D is a $[\overline{1}36]$ 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

$$
\begin{array}{ccc}
\bar{X} & \bar{Y} & \bar{Z} \\
\frac{a}{6} & \frac{b}{2} & -c \\
\frac{1}{6} & \frac{1}{2} & -1 \\
\end{array}
$$

Projections in terms of $a$, $b$, and $c$

Reduction to integers

Enclosure $[\overline{1}36]$
14. Do you expect gold and silver to have the same (a) atomic packing factor, (b) volume of unit cell, (c) number of atoms per unit cells, and (d) coordination number? Verify your answer.

Answer:

We expect gold and silver, both FCC, to have the same atomic packing factor (0.74), # of atoms per unit cell (4), and coordination # (12).

The volume of the cell will be larger for the atom with the larger atomic radius. (Refer to Table 3.3 for verification)