4.3 Calculate the activation energy for vacancy formation in aluminum, given that the equilibrium number of vacancies at 500 °C (773 K) is  $7.57 \times 10^{23}$  m<sup>-3</sup>. The atomic weight and density (at 500 °C) for aluminum are, respectively, 26.98 g/mol and 2.62 g/cm<sup>3</sup>.

## Solution

Upon examination of Equation 4.1, all parameters besides  $Q_{\nu}$  are given except N, the total number of atomic sites. However, N is related to the density,  $(\rho_{Al})$ , Avogadro's number  $(N_A)$ , and the atomic weight  $(A_{Al})$  according to Equation 4.2 as

$$N = \frac{N_{\rm A} \rho_{\rm Al}}{A_{\rm Al}}$$

$$= \frac{(6.022 \times 10^{23} \text{ atoms/mol})(2.62 \text{ g/cm}^3)}{26.98 \text{ g/mol}}$$

$$= 5.85 \times 10^{22} \text{ atoms/cm}^3 = 5.85 \times 10^{28} \text{ atoms/m}^3$$

Now, taking natural logarithms of both sides of Equation 4.1,

$$\ln N_{v} = \ln N - \frac{Q_{v}}{kT}$$

and, after some algebraic manipulation

$$Q_{v} = -kT \ln \left( \frac{N_{v}}{N} \right)$$

= 
$$-(8.62 \times 10^{-5} \text{ eV/atom} - \text{K})(500^{\circ}\text{C} + 273 \text{ K}) \ln \left[ \frac{7.57 \times 10^{23} \text{ m}^{-3}}{5.85 \times 10^{28} \text{ m}^{-3}} \right]$$

$$= 0.75 \text{ eV/atom}$$

4.4 Below, atomic radius, crystal structure, electronegativity, and the most common valence are tabulated, for several elements; for those that are nonmetals, only atomic radii are indicated.

	( <i>nm</i> )	Crystal Structure	Electronegativity	Valence
Cu	0.1278	FCC	1.9	+2
С	0.071			
Н	0.046			
0	0.060			
Ag	0.1445	FCC	1.9	+1
Al	0.1431	FCC	1.5	+3
Со	0.1253	НСР	1.8	+2
Cr	0.1249	ВСС	1.6	+3
Fe	0.1241	ВСС	1.8	+2
Ni	0.1246	FCC	1.8	+2
Pd	0.1376	FCC	2.2	+2
Pt	0.1387	FCC	2.2	+2
Zn	0.1332	НСР	1.6	+2

Which of these elements would you expect to form the following with copper:

## Solution

<sup>(</sup>a) A substitutional solid solution having complete solubility

<sup>(</sup>b) A substitutional solid solution of incomplete solubility

<sup>(</sup>c) An interstitial solid solution

In this problem we are asked to cite which of the elements listed form with Cu the three possible solid solution types. For complete substitutional solubility the following criteria must be met: 1) the difference in atomic radii between Cu and the other element ( $\Delta R\%$ ) must be less than  $\pm 15\%$ , 2) the crystal structures must be the same, 3) the electronegativities must be similar, and 4) the valences should be the same, or nearly the same. Below are tabulated, for the various elements, these criteria.

Element	<u>ΔR%</u>	Crystal <u>Structure</u>	ΔElectro- negativity	<u>Valence</u>
Cu		FCC		2+
C	-44			
Н	-64			
O	-53			
Ag	+13	FCC	0	1+
Al	+12	FCC	-0.4	3+
Co	-2	HCP	-0.1	2+
Cr	-2	BCC	-0.3	3+
Fe	-3	BCC	-0.1	2+
Ni	-3	FCC	-0.1	2+
Pd	+8	FCC	+0.3	2+
Pt	+9	FCC	+0.3	2+
Zn	+4	HCP	-0.3	2+

- (a) Ni, Pd, and Pt meet all of the criteria and thus form substitutional solid solutions having complete solubility. At elevated temperatures Co and Fe experience allotropic transformations to the FCC crystal structure, and thus display complete solid solubility at these temperatures.
- (b) Ag, Al, Co, Cr, Fe, and Zn form substitutional solid solutions of incomplete solubility. All these metals have either BCC or HCP crystal structures, and/or the difference between their atomic radii and that for Cu are greater than  $\pm 15\%$ , and/or have a valence different than 2+.
- (c) **C, H, and O form interstitial solid solutions**. These elements have atomic radii that are significantly smaller than the atomic radius of Cu.

4.8 What is the composition, in weight percent, of an alloy that consists of 6 at% Pb and 94 at% Sn?

# Solution

In order to compute composition, in weight percent, of a 6 at% Pb-94 at% Sn alloy, we employ Equation 4.7 as

$$C_{Pb} = \frac{C'_{Pb}A_{Pb}}{C'_{Pb}A_{Pb} + C'_{Sn}A_{Sn}} \times 100$$

$$= \frac{(6)(207.2 \text{ g/mol})}{(6)(207.2 \text{ g/mol}) + (94)(118.71 \text{ g/mol})} \times 100$$

$$= 10.0 \text{ wt\%}$$

$$C_{\text{Sn}} = \frac{C_{\text{Sn}}' A_{\text{Sn}}}{C_{\text{Pb}}' A_{\text{Pb}} + C_{\text{Sn}}' A_{\text{Sn}}} \times 100$$

$$= \frac{(94)(118.71 \text{ g/mol})}{(6)(207.2 \text{ g/mol}) + (94)(118.71 \text{ g/mol})} \times 100$$

= 90.0 wt%

4.18 Some hypothetical alloy is composed of 12.5 wt% of metal A and 87.5 wt% of metal B. If the densities of metals A and B are 4.27 and 6.35 g/cm³, respectively, whereas their respective atomic weights are 61.4 and 125.7 g/mol, determine whether the crystal structure for this alloy is simple cubic, face-centered cubic, or body-centered cubic. Assume a unit cell edge length of 0.395 nm.

#### Solution

In order to solve this problem it is necessary to employ Equation 3.5; in this expression density and atomic weight will be averages for the alloy—that is

$$\rho_{\text{ave}} = \frac{nA_{\text{ave}}}{V_C N_A}$$

Inasmuch as for each of the possible crystal structures, the unit cell is cubic, then  $V_C = a^3$ , or

$$\rho_{\text{ave}} = \frac{nA_{\text{ave}}}{a^3N_{\Delta}}$$

And, in order to determine the crystal structure it is necessary to solve for n, the number of atoms per unit cell. For n = 1, the crystal structure is simple cubic, whereas for n values of 2 and 4, the crystal structure will be either BCC or FCC, respectively. When we solve the above expression for n the result is as follows:

$$n = \frac{\rho_{\text{ave}} a^3 N_{\text{A}}}{A_{\text{ave}}}$$

Expressions for  $A_{\text{ave}}$  and  $\rho_{\text{ave}}$  are found in Equations 4.11a and 4.10a, respectively, which, when incorporated into the above expression yields

$$n = \frac{\left(\frac{100}{\frac{C_{A}}{\rho_{A}} + \frac{C_{B}}{\rho_{B}}}\right) a^{3} N_{A}}{\left(\frac{100}{\frac{C_{A}}{A_{A}} + \frac{C_{B}}{A_{B}}}\right)}$$

Substitution of the concentration values (i.e.,  $C_{\rm A}$  = 12.5 wt% and  $C_{\rm B}$  = 87.5 wt%) as well as values for the other parameters given in the problem statement, into the above equation gives

$$n = \frac{\left(\frac{100}{\frac{12.5 \text{ wt\%}}{4.27 \text{ g/cm}^3} + \frac{87.5 \text{ wt\%}}{6.35 \text{ g/cm}^3}}\right) (3.95 \times 10^{-8} \text{ nm})^3 (6.022 \times 10^{23} \text{ atoms/mol})}{\left(\frac{100}{\frac{12.5 \text{ wt\%}}{61.4 \text{ g/mol}} + \frac{87.5 \text{ wt\%}}{125.7 \text{ g/mol}}\right)}$$

= 2.00 atoms/unit cell

Therefore, on the basis of this value, the crystal structure is body-centered cubic.

4.35 Determine the ASTM grain size number if 25 grains per square inch are measured at a magnification of 600.

## Solution

This problem asks that we determine the ASTM grain size number if 8 grains per square inch are measured at a magnification of 600. In order to solve this problem we make use of Equation 4.17:

$$N_M \left(\frac{M}{100}\right)^2 = 2^{n-1}$$

where  $N_M$  = the number of grains per square inch at magnification M, and n is the ASTM grain size number. Solving the above equation for n, and realizing that  $N_M$  = 8, while M = 600, we have

$$n = \frac{\log N_M + 2 \log \left(\frac{M}{100}\right)}{\log 2} + 1$$

$$= \frac{\log 8 + 2 \log \left(\frac{600}{100}\right)}{\log 2} + 1 = 9.2$$