CHAPTER 4

IMPERFECTIONS IN SOLIDS

PROBLEM SOLUTIONS

Vacancies and Self-Interstitials

4.1 In order to compute the fraction of atom sites that are vacant in copper at 1357 K, we must employ Equation 4.1. As stated in the problem, $Q_v = 0.90 \text{ eV}/\text{atom}$. Thus,

$$\frac{N_{\nu}}{N} = \exp\left(-\frac{Q_{\nu}}{kT}\right) = \exp\left[-\frac{0.90 \text{ eV/atom}}{(8.62 \times 10^{-5} \text{ eV/atom} - \text{K})(1357 \text{ K})}\right]$$

 $= 4.56 \times 10^{-4}$

4.2 Determination of the number of vacancies per cubic meter in gold at 900°C (1173 K) requires the utilization of Equations 4.1 and 4.2 as follows:

$$N_{v} = N \exp\left(-\frac{Q_{v}}{kT}\right) = \frac{N_{A}\rho_{Au}}{A_{Au}} \exp\left(-\frac{Q_{v}}{kT}\right)$$
$$= \frac{(6.023 \times 10^{23} \text{ atoms/mol})(18.63 \text{ g/cm}^{3})}{196.9 \text{ g/mol}} \exp\left[-\frac{0.98 \text{ eV/atom}}{(8.62 \times 10^{-5} \text{ eV/atom}-\text{K})(1173 \text{ K})}\right]$$

$$= 3.52 \text{ x } 10^{18} \text{ cm}^{-3} = 3.52 \text{ x } 10^{24} \text{ m}^{-3}$$

4.3 This problem calls for the computation of the activation energy for vacancy formation in silver. Upon examination of Equation 4.1, all parameters besides Q_v are given except *N*, the total number of atomic sites. However, *N* is related to the density, (ρ), Avogadro's number (N_A), and the atomic weight (*A*) according to Equation 4.2 as

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

$$= \frac{(6.023 \times 10^{23} \text{ atoms/mol})(9.5 \text{ g/cm}^3)}{107.9 \text{ g/mol}}$$

 $= 5.30 \text{ x } 10^{22} \text{ atoms/cm}^3 = 5.30 \text{ x } 10^{28} \text{ atoms/m}^3$

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

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

$$= - (8.62 \times 10^{-5} \text{ eV/atom-K})(800^{\circ}\text{C} + 273 \text{ K}) \ln \left[\frac{3.60 \times 10^{23} \text{ m}^{-3}}{5.30 \times 10^{28} \text{ m}^{-3}}\right]$$

= 1.10 eV/atom

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Impurities in Solids

4.4 In this problem we are asked to cite which of the elements listed form with Ni the three possible solid solution types. For complete substitutional solubility the following criteria must be met: 1) the difference in atomic radii between Ni and the other element (ΔR %) must be less than ±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 | $\Delta R\%$ | Crystal <u>Structure</u> | ∆Electro- negativity | Valence |
|---------|--------------|-----------------------------|-------------------------|---------|
| Ni | | FCC | | 2+ |
| С | -43 | | | |
| Н | -63 | | | |
| 0 | -52 | | | |
| Ag | +16 | FCC | +0.1 | 1+ |
| Al | +15 | FCC | -0.3 | 3+ |
| Co | +0.6 | HCP | 0 | 2+ |
| Cr | +0.2 | BCC | -0.2 | 3+ |
| Fe | -0.4 | BCC | 0 | 2+ |
| Pt | +11 | FCC | +0.4 | 2+ |
| Zn | +7 | HCP | -0.2 | 2+ |

(a) Pt is the only element that meets all of the criteria and thus forms a substitutional solid solution 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 Ni 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 Ni.

4.5 In the drawing below is shown the atoms on the (100) face of an FCC unit cell; the interstitial site is at the center of the edge.



The diameter of an atom that will just fit into this site (2r) is just the difference between that unit cell edge length (*a*) and the radii of the two host atoms that are located on either side of the site (*R*); that is

$$2r = a - 2R$$

However, for FCC *a* is related to *R* according to Equation 3.1 as $a = 2R\sqrt{2}$; therefore, solving for *r* from the above equation gives

$$r = \frac{a-2R}{2} = \frac{2R\sqrt{2}-2R}{2} = 0.41R$$

A (100) face of a BCC unit cell is shown below.



The interstitial atom that just fits into this interstitial site is shown by the small circle. It is situated in the plane of this (100) face, midway between the two vertical unit cell edges, and one quarter of the distance between the bottom and top cell edges. From the right triangle that is defined by the three arrows we may write

$$\left(\frac{a}{2}\right)^2 + \left(\frac{a}{4}\right)^2 = (R+r)^2$$

However, from Equation 3.3, $a = \frac{4R}{\sqrt{3}}$, and, therefore, making this substitution, the above equation takes the form

$$\left(\frac{4R}{2\sqrt{3}}\right)^2 + \left(\frac{4R}{4\sqrt{3}}\right)^2 = R^2 + 2Rr + r^2$$

After rearrangement the following quadratic equation results:

$$r^2 + 2Rr - 0.667R^2 = 0$$

And upon solving for *r*:

$$r = \frac{-(2R) \pm \sqrt{(2R)^2 - (4)(1)(-0.667R^2)}}{2}$$

$$= \frac{-2R \pm 2.582R}{2}$$

And, finally

$$r(+) = \frac{-2R + 2.582R}{2} = 0.291R$$
$$r(-) = \frac{-2R - 2.582R}{2} = -2.291R$$

Of course, only the r(+) root is possible, and, therefore, r = 0.291R.

Thus, for a host atom of radius R, the size of an interstitial site for FCC is approximately 1.4 times that for BCC.

Specification of Composition

4.6 (a) This problem asks that we derive Equation 4.7a. To begin, C_1 is defined according to Equation 4.3 as

$$C_1 = \frac{m_1}{m_1 + m_2} \times 100$$

or, equivalently

$$C_1 = \frac{m'_1}{m'_1 + m'_2} \times 100$$

where the primed m's indicate masses in grams. From Equation 4.4 we may write

$$m_1' = n_{m1} A_1$$
$$m_2' = n_{m2} A_2$$

And, substitution into the C_1 expression above

$$C_1 = \frac{n_{m1}A_1}{n_{m1}A_1 + n_{m2}A_2} \times 100$$

From Equation 4.5 it is the case that

$$n_{m1} = \frac{C_1'(n_{m1} + n_{m2})}{100}$$

$$n_{m2} = \frac{C_2'(n_{m1} + n_{m2})}{100}$$

And substitution of these expressions into the above equation leads to

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$$C_1 = \frac{C_1'A_1}{C_1'A_1 + C_2'A_2} \times 100$$

which is just Equation 4.7a.

(b) This problem asks that we derive Equation 4.9a. To begin, $C_1^{"}$ is defined as the mass of component 1 per unit volume of alloy, or

$$C_1'' = \frac{m_1}{V}$$

If we assume that the total alloy volume V is equal to the sum of the volumes of the two constituents--i.e., $V = V_1 + V_2$ --then

$$C_1'' = \frac{m_1}{V_1 + V_2}$$

Furthermore, the volume of each constituent is related to its density and mass as

$$V_1 = \frac{m_1}{\rho_1}$$
$$V_2 = \frac{m_2}{\rho_2}$$

This leads to

$$C_{1}'' = \frac{m_{1}}{\frac{m_{1}}{\rho_{1}} + \frac{m_{2}}{\rho_{2}}}$$

From Equation 4.3, m_1 and m_2 may be expressed as follows:

$$m_1 = \frac{C_1(m_1 + m_2)}{100}$$

$$m_2 = \frac{C_2 (m_1 + m_2)}{100}$$

Substitution of these equations into the preceding expression yields

$$C_{1}^{"} = \frac{\frac{C_{1}(m_{1} + m_{2})}{100}}{\frac{C_{1}(m_{1} + m_{2})}{\rho_{1}}} + \frac{\frac{C_{2}(m_{1} + m_{2})}{100}}{\rho_{2}}$$
$$= \frac{C_{1}}{\frac{C_{1}}{\rho_{1}} + \frac{C_{2}}{\rho_{2}}}$$

If the densities ρ_1 and ρ_2 are given in units of g/cm³, then conversion to units of kg/m³ requires that we multiply this equation by 10^3 , inasmuch as

$$1 \text{ g/cm}^3 = 10^3 \text{ kg/m}^3$$

Therefore, the previous equation takes the form

$$C_1'' = \frac{C_1}{\frac{C_1}{\rho_1} + \frac{C_2}{\rho_2}} \times 10^3$$

which is the desired expression.

(c) Now we are asked to derive Equation 4.10a. The density of an alloy ρ_{ave} is just the total alloy mass *M* divided by its volume *V*

$$\rho_{\text{ave}} = \frac{M}{V}$$

Or, in terms of the component elements 1 and 2

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[*Note:* here it is assumed that the total alloy volume is equal to the separate volumes of the individual components, which is only an approximation; normally V will not be exactly equal to $(V_1 + V_2)$]. Each of V_1 and V_2 may be expressed in terms of its mass and density as,

$$V_1 = \frac{m_1}{\rho_1}$$
$$V_2 = \frac{m_2}{\rho_2}$$

100

When these expressions are substituted into the above equation, we get

$$\rho_{\text{ave}} = \frac{m_1 + m_2}{\frac{m_1}{\rho_1} + \frac{m_2}{\rho_2}}$$

Furthermore, from Equation 4.3

$$m_1 = \frac{C_1(m_1 + m_2)}{100}$$
$$m_2 = \frac{C_2(m_1 + m_2)}{100}$$

Which, when substituted into the above ρ_{ave} expression yields

$$\rho_{\text{ave}} = \frac{\frac{m_1 + m_2}{C_1(m_1 + m_2)}}{\frac{100}{\rho_1} + \frac{C_2(m_1 + m_2)}{\frac{100}{\rho_2}}}$$

And, finally, this equation reduces to

$$= \frac{100}{\frac{C_1}{\rho_1} + \frac{C_2}{\rho_2}}$$

4.7 In order to compute composition, in atom percent, of a 92.5 wt% Ag-7.5 wt% Cu alloy, we employ Equation 4.6 as

$$C'_{\text{Ag}} = \frac{C_{\text{Ag}}A_{\text{Cu}}}{C_{\text{Ag}}A_{\text{Cu}} + C_{\text{Cu}}A_{\text{Ag}}} \times 100$$

$$= \frac{(92.5)(63.55 \text{ g/mol})}{(92.5)(63.55 \text{ g/mol}) + (7.5)(107.87 \text{g/mol})} \times 100$$

$$C'_{\rm Cu} = \frac{C_{\rm Cu}A_{\rm Ag}}{C_{\rm Ag}A_{\rm Cu} + C_{\rm Cu}A_{\rm Ag}} \times 100$$

$$= \frac{(7.5)(107.87 \text{ g/mol})}{(92.5)(63.55 \text{ g/mol}) + (7.5)(107.87 \text{g/mol})} \times 100$$

= 12.1 at%

4.8 In order to compute composition, in weight percent, of a 5 at% Cu-95 at% Pt alloy, we employ Equation 4.7 as

$$C_{\text{Cu}} = \frac{C_{\text{Cu}}' A_{\text{Cu}}}{C_{\text{Cu}}' A_{\text{Cu}} + C_{\text{Pt}}' A_{\text{Pt}}} \times 100$$

$$= \frac{(5)(63.55 \text{ g/mol})}{(5)(63.55 \text{ g/mol}) + (95)(195.08 \text{ g/mol})} \times 100$$

$$= 1.68 \text{ wt\%}$$

$$C_{\text{Pt}} = \frac{C_{\text{Pt}}'A_{\text{Pt}}}{C_{\text{Cu}}'A_{\text{Cu}} + C_{\text{Pt}}'A_{\text{Pt}}} \times 100$$

 $= \frac{(95)(195.08 \text{ g/mol})}{(5)(63.55 \text{ g/mol}) + (95)(195.08 \text{ g/mol})} \times 100$

= 98.32 wt%

4.9 The concentration, in weight percent, of an element in an alloy may be computed using a modified form of Equation 4.3. For this alloy, the concentration of iron (C_{Fe}) is just

$$C_{\text{Fe}} = \frac{m_{\text{Fe}}}{m_{\text{Fe}} + m_{\text{C}} + m_{\text{Cr}}} \times 100$$
$$= \frac{105 \text{ kg}}{105 \text{ kg} + 0.2 \text{ kg} + 1.0 \text{ kg}} \times 100 = 98.87 \text{ wt\%}$$

Similarly, for carbon

$$C_{\rm C} = \frac{0.2 \text{ kg}}{105 \text{ kg} + 0.2 \text{ kg} + 1.0 \text{ kg}} \times 100 = 0.19 \text{ wt}\%$$

And for chromium

$$C_{\rm Cr} = \frac{1.0 \text{ kg}}{105 \text{ kg} + 0.2 \text{ kg} + 1.0 \text{ kg}} \times 100 = 0.94 \text{ wt\%}$$

4.10 The concentration of an element in an alloy, in atom percent, may be computed using Equation 4.5. However, it first becomes necessary to compute the number of moles of both Cu and Zn, using Equation 4.4. Thus, the number of moles of Cu is just

$$n_{m_{\text{Cu}}} = \frac{m_{\text{Cu}}}{A_{\text{Cu}}} = \frac{33 \text{ g}}{63.55 \text{ g/mol}} = 0.519 \text{ mol}$$

Likewise, for Zn

$$n_{m_{Zn}} = \frac{47 \text{ g}}{65.39 \text{ g/mol}} = 0.719 \text{ mol}$$

Now, use of Equation 4.5 yields

$$C_{\rm Cu} = \frac{n_{m_{\rm Cu}}}{n_{m_{\rm Cu}} + n_{m_{\rm Zn}}} \times 100$$

$$= \frac{0.519 \text{ mol}}{0.519 \text{ mol} + 0.719 \text{ mol}} \times 100 = 41.9 \text{ at\%}$$

Also,

$$C'_{\text{Zn}} = \frac{0.719 \text{ mol}}{0.519 \text{ mol} + 0.719 \text{ mol}} \times 100 = 58.1 \text{ at\%}$$

4.11 In this problem we are asked to determine the concentrations, in atom percent, of the Ag-Au-Cu alloy. It is first necessary to convert the amounts of Ag, Au, and Cu into grams.

$$m'_{Ag} = (44.5 \text{ lb}_{m})(453.6 \text{ g/lb}_{m}) = 20,185 \text{ g}$$

 $m'_{Au} = (83.7 \text{ lb}_{m})(453.6 \text{ g/lb}_{m}) = 37,966 \text{ g}$
 $m'_{Cu} = (5.3 \text{ lb}_{m})(453.6 \text{ g/lb}_{m}) = 2,404 \text{ g}$

These masses must next be converted into moles (Equation 4.4), as

$$n_{m_{Ag}} = \frac{m_{Ag}}{A_{Ag}} = \frac{20,185 \text{ g}}{107.87 \text{ g/mol}} = 187.1 \text{ mol}$$
$$n_{m_{Au}} = \frac{37,966 \text{ g}}{196.97 \text{ g/mol}} = 192.8 \text{ mol}$$
$$n_{m_{Cu}} = \frac{2,404 \text{ g}}{63.55 \text{ g/mol}} = 37.8 \text{ mol}$$

Now, employment of a modified form of Equation 4.5, gives

$$C'_{Ag} = \frac{n_{m_{Ag}}}{n_{m_{Ag}} + n_{m_{Au}} + n_{m_{Cu}}} \times 100$$

$$= \frac{187.1 \text{ mol}}{187.1 \text{ mol} + 192.8 \text{ mol} + 37.8 \text{ mol}} \times 100 = 44.8 \text{ at\%}$$

$$C'_{Au} = \frac{192.8 \text{ mol}}{187.1 \text{ mol} + 192.8 \text{ mol} + 37.8 \text{ mol}} \times 100 = 46.2 \text{ at\%}$$

$$C_{\rm Cu} = \frac{37.8 \text{ mol}}{187.1 \text{ mol} + 192.8 \text{ mol} + 37.8 \text{ mol}} \times 100 = 9.0 \text{ at}\%$$

4.12 We are asked to compute the composition of a Pb-Sn alloy in atom percent. Employment of Equation4.6 leads to

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

$$\frac{5.5(118.69 \text{ g/mol})}{5.5(118.69 \text{ g/mol}) + 94.5(207.2 \text{ g/mol})} \times 100$$

=

= 3.2 at%

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

$$= \frac{94.5(207.2 \text{ g/mol})}{94.5(207.2 \text{ g/mol}) + 5.5(118.69 \text{ g/mol})} \times 100$$

= 96.8 at%

4-19

4.13 This problem calls for a conversion of composition in atom percent to composition in weight percent. The composition in atom percent for Problem 4.11 is 44.8 at% Ag, 46.2 at% Au, and 9.0 at% Cu. Modification of Equation 4.7 to take into account a three-component alloy leads to the following

$$C_{\text{Ag}} = \frac{C'_{\text{Ag}}A_{\text{Ag}}}{C'_{\text{Ag}}A_{\text{Ag}} + C'_{\text{Au}}A_{\text{Au}} + C'_{\text{Cu}}A_{\text{Cu}}} \times 100$$

 $= \frac{(44.8)(107.87 \text{ g/mol})}{(44.8)(107.87 \text{ g/mol}) + (46.2)(196.97 \text{ g/mol}) + (9.0)(63.55 \text{ g/mol})} \times 100$

$$C_{Au} = \frac{C'_{Au}A_{Au}}{C'_{Ag}A_{Ag} + C'_{Au}A_{Au} + C'_{Cu}A_{Cu}} \times 100$$

.

$$= \frac{(46.2)(196.97 \text{ g/mol})}{(44.8)(107.87 \text{ g/mol}) + (46.2)(196.97 \text{ g/mol}) + (9.0)(63.55 \text{ g/mol})} \times 100$$

$$C_{\rm Cu} = \frac{C'_{\rm Cu}A_{\rm Cu}}{C'_{\rm Ag}A_{\rm Ag} + C'_{\rm Au}A_{\rm Au} + C'_{\rm Cu}A_{\rm Cu}} \times 100$$

$$\frac{(9.0)(63.55 \text{ g/mol})}{(44.8)(107.87 \text{ g/mol}) + (46.2)(196.97 \text{ g/mol}) + (9.0)(63.55 \text{ g/mol})} \times 100$$

=

$$= 4.0 \text{ wt\%}$$

4.14 This problem calls for a determination of the number of atoms per cubic meter for lead. In order to solve this problem, one must employ Equation 4.2,

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

The density of Pb (from the table inside of the front cover) is 11.35 g/cm^3 , while its atomic weight is 207.2 g/mol. Thus,

$$N = \frac{(6.023 \text{ x } 10^{23} \text{ atoms/mol})(11.35 \text{ g/cm}^3)}{207.2 \text{ g/mol}}$$

$$= 3.30 \times 10^{22} \text{ atoms/cm}^3 = 3.30 \times 10^{28} \text{ atoms/m}^3$$

4.15 In order to compute the concentration in kg/m^3 of Si in a 0.25 wt% Si-99.75 wt% Fe alloy we must employ Equation 4.9 as

$$C_{\rm Si}^{"} = \frac{C_{\rm Si}}{\frac{C_{\rm Si}}{\rho_{\rm Si}} + \frac{C_{\rm Fe}}{\rho_{\rm Fe}}} \times 10^3$$

From inside the front cover, densities for silicon and iron are 2.33 and 7.87 g/cm³, respectively; and, therefore

$$C_{\rm Si}^{"} = \frac{0.25}{\frac{0.25}{2.33 \text{ g/cm}^3} + \frac{99.75}{7.87 \text{ g/cm}^3}} \times 10^3$$

$$= 19.6 \text{ kg/m}^3$$

4.16 We are asked in this problem to determine the approximate density of a Ti-6Al-4V titanium alloy that has a composition of 90 wt% Ti, 6 wt% Al, and 4 wt% V. In order to solve this problem, Equation 4.10a is modified to take the following form:

$$\rho_{\text{ave}} = \frac{100}{\frac{C_{\text{Ti}}}{\rho_{\text{Ti}}} + \frac{C_{\text{Al}}}{\rho_{\text{Al}}} + \frac{C_{\text{V}}}{\rho_{\text{V}}}}$$

And, using the density values for Ti, Al, and V—i.e., 4.51 g/cm^3 , 2.71 g/cm^3 , and 6.10 g/cm^3 —(as taken from inside the front cover of the text), the density is computed as follows:

$$\rho_{\text{ave}} = \frac{100}{\frac{90 \text{ wt\%}}{4.51 \text{ g/cm}^3} + \frac{6 \text{ wt\%}}{2.71 \text{ g/cm}^3} + \frac{4 \text{ wt\%}}{6.10 \text{ g/cm}^3}}$$

$$= 4.38 \text{ g/cm}^{3}$$

4.17 This problem asks that we determine the unit cell edge length for a 80 wt% Ag-20 wt% Pd alloy. 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 the unit cell is cubic, then $V_C = a^3$, then

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

And solving this equation for the unit cell edge length, leads to

$$a = \left(\frac{nA_{\text{ave}}}{\rho_{\text{ave}}N_{\text{A}}}\right)^{1/3}$$

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

$$a = \left[\frac{n \left(\frac{100}{\frac{C_{Ag}}{A_{Ag}} + \frac{C_{Pd}}{A_{Pd}}} \right)}{\left(\frac{100}{\frac{C_{Ag}}{\rho_{Ag}} + \frac{C_{Pd}}{\rho_{Pd}}} \right)^{N_{A}}} \right]^{1/3}$$

Since the crystal structure is FCC, the value of n in the above expression is 4 atoms per unit cell. The atomic weights for Ag and Pd are 107.9 and 106.4 g/mol, respectively (Figure 2.6), whereas the densities for the Ag and Pd are 10.49 g/cm³ (inside front cover) and 12.02 g/cm³. Substitution of these, as well as the concentration values stipulated in the problem statement, into the above equation gives

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$$a = \begin{bmatrix} (4 \text{ atoms/unit cell}) \left(\frac{100}{\frac{80 \text{ wt\%}}{107.9 \text{ g/mol}} + \frac{20 \text{ wt\%}}{106.4 \text{ g/mol}}} \right) \\ \left(\frac{100}{\frac{80 \text{ wt\%}}{10.49 \text{ g/cm}^3} + \frac{20 \text{ wt\%}}{12.02 \text{ g/cm}^3}} \right) (6.023 \times 10^{23} \text{ atoms/mol}) \end{bmatrix}$$

= 4.050×10^{-8} cm = 0.4050 nm

4.18 This problem asks that we determine, for a hypothetical alloy that is composed of 25 wt% of metal A and 75 wt% of metal B, whether the crystal structure is simple cubic, face-centered cubic, or body-centered cubic. We are given the densities of the these metals ($\rho_A = 6.17 \text{ g/cm}^3$ and $\rho_B = 8.00 \text{ g/cm}^3$ for B), their atomic weights ($A_A = 171.3 \text{ g/mol}$ and $A_B = 162.0 \text{ g/mol}$), and that the unit cell edge length is 0.332 nm (i.e., 3.32 x 10⁻⁸ cm). 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

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

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:

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

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

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

Substitution of the concentration values (i.e., $C_A = 25$ wt% and $C_B = 75$ wt%) as well as values for the other parameters given in the problem statement, into the above equation gives

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$$n = \frac{\left(\frac{100}{\frac{25 \text{ wt\%}}{6.17 \text{ g/cm}^3} + \frac{75 \text{ wt\%}}{8.00 \text{ g/cm}^3}}\right)^{(3.32 \times 10^{-8} \text{ nm})^3(6.023 \times 10^{23} \text{ atoms/mol})}}{\left(\frac{100}{\frac{25 \text{ wt\%}}{171.3 \text{ g/mol}} + \frac{75 \text{ wt\%}}{162.0 \text{ g/mol}}}\right)}$$

= 1.00 atom/unit cell

Therefore, on the basis of this value, the crystal structure is simple cubic.

4.19 This problem asks that we derive Equation 4.18, using other equations given in the chapter. The concentration of component 1 in atom percent (C'_1) is just $100 c'_1$ where c'_1 is the atom fraction of component 1. Furthermore, c'_1 is defined as $c'_1 = N_1/N$ where N_1 and N are, respectively, the number of atoms of component 1 and total number of atoms per cubic centimeter. Thus, from the above discussion the following holds:

$$N_1 = \frac{C_1' N}{100}$$

Substitution into this expression of the appropriate form of N from Equation 4.2 yields

$$N_1 = \frac{C_1 N_A \rho_{\text{ave}}}{100 A_{\text{ave}}}$$

And, finally, substitution into this equation expressions for C_1' (Equation 4.6a), ρ_{ave} (Equation 4.10a), A_{ave} (Equation 4.11a), and realizing that $C_2 = (C_1 - 100)$, and after some algebraic manipulation we obtain the desired expression:

$$N_{1} = \frac{N_{A}C_{1}}{\frac{C_{1}A_{1}}{\rho_{1}} + \frac{A_{1}}{\rho_{2}}(100 - C_{1})}$$

4.20 This problem asks us to determine the number of molybdenum atoms per cubic centimeter for a 16.4 wt% Mo-83.6 wt% W solid solution. To solve this problem, employment of Equation 4.18 is necessary, using the following values:

$$C_1 = C_{Mo} = 16.4 \text{ wt\%}$$

 $\rho_1 = \rho_{Mo} = 10.22 \text{ g/cm}^3$
 $\rho_2 = \rho_W = 19.3 \text{ g/cm}^3$
 $A_1 = A_{Mo} = 95.94 \text{ g/mol}$

Thus

$$N_{\rm Mo} = \frac{N_{\rm A} C_{\rm Mo}}{\frac{C_{\rm Mo} A_{\rm Mo}}{\rho_{\rm Mo}} + \frac{A_{\rm Mo}}{\rho_{\rm W}} (100 - C_{\rm Mo})}$$

$$= \frac{(6.023 \times 10^{23} \text{ atoms/mol}) (16.4 \text{ wt\%})}{\frac{(16.4 \text{ wt\%})(95.94 \text{ g/mol})}{10.22 \text{ g/cm}^3} + \frac{95.94 \text{ g/mol}}{19.3 \text{ g/cm}^3} (100 - 16.4 \text{ wt\%})}$$

$$= 1.73 \text{ x } 10^{22} \text{ atoms/cm}^3$$

4.21 This problem asks us to determine the number of niobium atoms per cubic centimeter for a 24 wt% Nb-76 wt% V solid solution. To solve this problem, employment of Equation 4.18 is necessary, using the following values:

$$C_1 = C_{Nb} = 24 \text{ wt\%}$$

 $\rho_1 = \rho_{Nb} = 8.57 \text{ g/cm}^3$
 $\rho_2 = \rho_V = 6.10 \text{ g/cm}^3$
 $A_1 = A_{Nb} = 92.91 \text{ g/mol}$

Thus

$$N_{\rm Nb} = \frac{N_{\rm A}C_{\rm Nb}}{\frac{C_{\rm Nb}A_{\rm Nb}}{\rho_{\rm Nb}} + \frac{A_{\rm Nb}}{\rho_{\rm V}}(100 - C_{\rm Nb})}$$

$$= \frac{(6.023 \times 10^{23} \text{ atoms/mol})(24 \text{ wt\%})}{\frac{(24 \text{ wt\%})(92.91 \text{ g/mol})}{8.57 \text{ g/cm}^3} + \frac{92.91 \text{ g/mol}}{6.10 \text{ g/cm}^3}(100 - 24 \text{ wt\%})}$$

$$= 1.02 \text{ x } 10^{22} \text{ atoms/cm}^3$$

4.22 This problem asks that we derive Equation 4.19, using other equations given in the chapter. The number of atoms of component 1 per cubic centimeter is just equal to the atom fraction of component 1 (c'_1) times the total number of atoms per cubic centimeter in the alloy (*N*). Thus, using the equivalent of Equation 4.2, we may write

$$N_1 = c_1 N = \frac{c_1 N_A \rho_{ave}}{A_{ave}}$$

Realizing that

$$c_1' = \frac{C_1'}{100}$$

and

$$C_2' = 100 - C_1'$$

and substitution of the expressions for ρ_{ave} and A_{ave} , Equations 4.10b and 4.11b, respectively, leads to

$$N_{1} = \frac{c_{1} N_{A} \rho_{ave}}{A_{ave}}$$
$$N_{A} C_{1} \rho_{1} \rho_{2}$$

$$= \frac{11_{A} \rho_{1} \rho_{1} \rho_{2}}{C_{1}' \rho_{2} A_{1} + (100 - C_{1}') \rho_{1} A_{2}}$$

And, solving for C_1 '

$$C_{1} = \frac{100 N_{1} \rho_{1} A_{2}}{N_{A} \rho_{1} \rho_{2} - N_{1} \rho_{2} A_{1} + N_{1} \rho_{1} A_{2}}$$

Substitution of this expression for C_1 into Equation 4.7a, which may be written in the following form

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$$C_1 = \frac{C_1' A_1}{C_1' A_1 + C_2' A_2} \times 100$$

$$= \frac{C_1' A_1}{C_1' A_1} \times 100$$

yields

$$C_1 = \frac{100}{1 + \frac{N_A \rho_2}{N_1 A_1} - \frac{\rho_2}{\rho_1}}$$

the desired expression.

4.23 This problem asks us to determine the weight percent of Au that must be added to Ag such that the resultant alloy will contain 5.5 x 10^{21} Au atoms per cubic centimeter. To solve this problem, employment of Equation 4.19 is necessary, using the following values:

$$N_1 = N_{Au} = 5.5 \text{ x } 10^{21} \text{ atoms/cm}^3$$

 $\rho_1 = \rho_{Au} = 19.32 \text{ g/cm}^3$
 $\rho_2 = \rho_{Ag} = 10.49 \text{ g/cm}^3$
 $A_1 = A_{Au} = 196.97 \text{ g/mol}$
 $A_2 = A_{Ag} = 107.87 \text{ g/mol}$

Thus

$$C_{Au} = \frac{100}{1 + \frac{N_A \rho_{Ag}}{N_{Au} A_{Au}} - \frac{\rho_{Ag}}{\rho_{Au}}}$$

| _ | 100 | |
|-----|--|--------------------------|
| _ | $(6.023 \times 10^{23} \text{ atoms/mol})(10.49 \text{ g/cm}^3)$ | (10.49 g/cm^3) |
| 1 + | $(5.5 \times 10^{21} \text{ atoms/cm}^3)(196.97 \text{ g/mol})$ | (19.32 g/cm^3) |

= 15.9 wt%

4.24 This problem asks us to determine the weight percent of Ge that must be added to Si such that the resultant alloy will contain 2.43 $\times 10^{21}$ Ge atoms per cubic centimeter. To solve this problem, employment of Equation 4.19 is necessary, using the following values:

$$N_1 = N_{\text{Ge}} = 2.43 \text{ x } 10^{21} \text{ atoms/cm}^3$$

 $\rho_1 = \rho_{\text{Ge}} = 5.32 \text{ g/cm}^3$
 $\rho_2 = \rho_{\text{Si}} = 2.33 \text{ g/cm}^3$
 $A_1 = A_{\text{Ge}} = 72.64 \text{ g/mol}$
 $A_2 = A_{\text{Si}} = 28.09 \text{ g/mol}$

Thus

$$C_{\text{Ge}} = \frac{100}{1 + \frac{N_{\text{A}}\rho_{\text{Si}}}{N_{\text{Ge}}A_{\text{Ge}}} - \frac{\rho_{\text{Si}}}{\rho_{\text{Ge}}}}$$

| _ | | 100 | | |
|-------|-----|---|--|--|
| - 1 - | 1 ⊥ | $(6.023 \times 10^{23} \text{ atoms/mol})(2.33 \text{ g/cm}^3)$ | $\left(\frac{2.33 \text{ g/cm}^3}{\text{g/cm}^3}\right)$ | |
| | ΙT | $(2.43 \times 10^{21} \text{ atoms/cm}^3)(72.64 \text{ g/mol})$ | $\left(\frac{5.32 \text{ g/cm}^3}{5.32 \text{ g/cm}^3}\right)$ | |

= 11.7 wt%

4.25 This problems asks that we compute the unit cell edge length for a 90 wt% Fe-10 wt% V alloy. First of all, the atomic radii for Fe and V (using the table inside the front cover) are 0.124 and 0.132 nm, respectively. Also, using Equation 3.5 it is possible to compute the unit cell volume, and inasmuch as the unit cell is cubic, the unit cell edge length is just the cube root of the volume. However, it is first necessary to calculate the density and average atomic weight of this alloy using Equations 4.10a and 4.11a. Inasmuch as the densities of iron and vanadium are 7.87g/cm³ and 6.10 g/cm³, respectively, (as taken from inside the front cover), the average density is just

$$\rho_{\text{ave}} = \frac{100}{\frac{C_{\text{V}}}{\rho_{\text{V}}} + \frac{C_{\text{Fe}}}{\rho_{\text{Fe}}}}$$
$$= \frac{100}{\frac{10 \text{ wt\%}}{6.10 \text{ g/cm}^3} + \frac{90 \text{ wt\%}}{7.87 \text{ g/cm}^3}}$$
$$= 7.65 \text{ g/cm}^3$$

And for the average atomic weight

$$A_{\text{ave}} = \frac{100}{\frac{C_{\text{V}}}{A_{\text{V}}} + \frac{C_{\text{Fe}}}{A_{\text{Fe}}}}$$

| _ | 100 | | | | |
|---|-------|--------|----|-------|-------|
| - | 10 | wt% | - | 90 | wt% |
| | 50.94 | g/mole | 1- | 55.85 | g/mol |

= 55.32 g/mol

Now, V_C is determined from Equation 3.5 as

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

$$= \frac{(2 \text{ atoms/unit cell})(55.32 \text{ g/mol})}{(7.65 \text{ g/cm}^3)(6.023 \times 10^{23} \text{ atoms/mol})}$$

$$= 2.40 \text{ x } 10^{-23} \text{ cm}^3/\text{unit cell}$$

And, finally

$$a = (V_C)^{1/3}$$

=
$$(2.40 \times 10^{-23} \text{ cm}^3/\text{unit cell})^{1/3}$$

 $= 2.89 \text{ x } 10^{-8} \text{ cm} = 0.289 \text{ nm}$

Dislocations—Linear Defects

4.26 The Burgers vector and dislocation line are perpendicular for edge dislocations, parallel for screw dislocations, and neither perpendicular nor parallel for mixed dislocations.

Interfacial Defects

4.27 The surface energy for a crystallographic plane will depend on its packing density [i.e., the planar density (Section 3.11)]—that is, the higher the packing density, the greater the number of nearest-neighbor atoms, and the more atomic bonds in that plane that are satisfied, and, consequently, the lower the surface energy. From the solution to Problem 3.53, planar densities for FCC (100) and (111) planes are $\frac{1}{4R^2}$ and $\frac{1}{2R^2\sqrt{3}}$, respectively—

that is $\frac{0.25}{R^2}$ and $\frac{0.29}{R^2}$ (where *R* is the atomic radius). Thus, since the planar density for (111) is greater, it will have

the lower surface energy.

4.28 The surface energy for a crystallographic plane will depend on its packing density [i.e., the planar density (Section 3.11)]—that is, the higher the packing density, the greater the number of nearest-neighbor atoms, and the more atomic bonds in that plane that are satisfied, and, consequently, the lower the surface energy. From the solution to Problem 3.54, the planar densities for BCC (100) and (110) are $\frac{3}{16R^2}$ and $\frac{3}{8R^2\sqrt{2}}$, respectively—

that is $\frac{0.19}{R^2}$ and $\frac{0.27}{R^2}$. Thus, since the planar density for (110) is greater, it will have the lower surface energy.

4.29 (a) The surface energy will be greater than the grain boundary energy. For grain boundaries, some atoms on one side of a boundary will bond to atoms on the other side; such is not the case for surface atoms. Therefore, there will be fewer unsatisfied bonds along a grain boundary.

(b) The small-angle grain boundary energy is lower than for a high-angle one because more atoms bond across the boundary for the small-angle, and, thus, there are fewer unsatisfied bonds.

4.30 (a) A twin boundary is an interface such that atoms on one side are located at mirror image positions of those atoms situated on the other boundary side. The region on one side of this boundary is called a twin.

(b) Mechanical twins are produced as a result of mechanical deformation and generally occur in BCC and HCP metals. Annealing twins form during annealing heat treatments, most often in FCC metals.

4.31 (a) The interfacial defect that exists for this stacking sequence is a twin boundary, which occurs at the indicated position.



The stacking sequence on one side of this position is mirrored on the other side.

(b) The interfacial defect that exists within this FCC stacking sequence is a stacking fault, which occurs between the two lines.



Within this region, the stacking sequence is HCP.

Grain Size Determination

4.32 (a) This problem calls for a determination of the average grain size of the specimen which microstructure is shown in Figure 4.14(b). Seven line segments were drawn across the micrograph, each of which was 60 mm long. The average number of grain boundary intersections for these lines was 8.7. Therefore, the average line length intersected is just

$$\frac{60 \text{ mm}}{8.7} = 6.9 \text{ mm}$$

Hence, the average grain diameter, d, is

$$d = \frac{\text{ave. line length intersected}}{\text{magnification}} = \frac{6.9 \text{ mm}}{100} = 6.9 \times 10^{-2} \text{ mm}$$

(b) This portion of the problem calls for us to estimate the ASTM grain size number for this same material. The average grain size number, n, is related to the number of grains per square inch, N, at a magnification of 100x according to Equation 4.16. Inasmuch as the magnification is 100x, the value of N is measured directly from the micrograph, which is approximately 12 grains. In order to solve for n in Equation 4.16, it is first necessary to take logarithms as

$$\log N = (n - 1) \log 2$$

From which *n* equals

$$n = \frac{\log N}{\log 2} + 1$$
$$= \frac{\log 12}{\log 2} + 1 = 4.6$$

4.33 (a) This portion of the problem calls for a determination of the average grain size of the specimen which microstructure is shown in Figure 9.25(a). Seven line segments were drawn across the micrograph, each of which was 60 mm long. The average number of grain boundary intersections for these lines was 6.3. Therefore, the average line length intersected is just

$$\frac{60 \text{ mm}}{6.3} = 9.5 \text{ mm}$$

Hence, the average grain diameter, d, is

$$d = \frac{\text{ave. line length intersected}}{\text{magnification}} = \frac{9.5 \text{ mm}}{90} = 0.106 \text{ mm}$$

(b) This portion of the problem calls for us to estimate the ASTM grain size number for this same material. The average grain size number, n, is related to the number of grains per square inch, N, at a magnification of 100x according to Equation 4.16. However, the magnification of this micrograph is not 100x, but rather 90x. Consequently, it is necessary to use 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. Taking logarithms of both sides of this equation leads to the following:

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

Solving this expression for *n* gives

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

From Figure 9.25(a), N_M is measured to be approximately 4, which leads to

$$n = \frac{\log 4 + 2 \log \left(\frac{90}{100}\right)}{\log 2} + 1$$

= 2.7

4.34 (a) This part of problem asks that we compute the number of grains per square inch for an ASTM grain size of 6 at a magnification of 100x. All we need do is solve for the parameter N in Equation 4.16, inasmuch as n = 6. Thus

$$N = 2^{n-1}$$

= $2^{6-1} = 32$ grains/in.²

1

(b) Now it is necessary to compute the value of N for no magnification. In order to solve this problem it is necessary to use 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. Without any magnification, M in the above equation is 1, and therefore,

$$N_1 \left(\frac{1}{100}\right)^2 = 2^{6-1} = 32$$

And, solving for N_1 , $N_1 = 320,000$ grains/in.².

4.35 This problem asks that we determine the ASTM grain size number if 30 grains per square inch are measured at a magnification of 250. 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 = 30, while M = 250, we have

$$n = \frac{\log N_M + 2 \log \left(\frac{M}{100}\right)}{\log 2} + 1$$
$$= \frac{\log 30 + 2 \log \left(\frac{250}{100}\right)}{\log 2} + 1 = 2.5$$

4.36 This problem asks that we determine the ASTM grain size number if 25 grains per square inch are measured at a magnification of 75. In order to solve this problem we make use of Equation 4.17—viz.

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

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 $N_M = 25$, while M = 75, we have

$$n = \frac{\log N_M + 2 \log\left(\frac{M}{100}\right)}{\log 2} + 1$$
$$= \frac{\log 25 + 2 \log\left(\frac{75}{100}\right)}{\log 2} + 1 = 4.8$$

DESIGN PROBLEMS

Specification of Composition

4.D1 This problem calls for us to compute the concentration of lithium (in wt%) that, when added to aluminum, will yield a density of 2.47 g/cm³. Solution of this problem requires the use of Equation 4.10a, which takes the form

$$\rho_{\text{ave}} = \frac{100}{\frac{C_{\text{Li}}}{\rho_{\text{Li}}} + \frac{100 - C_{\text{Li}}}{\rho_{\text{Al}}}}$$

inasmuch as $C_{\text{Li}} + C_{\text{Al}} = 100$. According to the table inside the front cover, the respective densities of Li and Al are 0.534 and 2.71 g/cm³. Upon solving for C_{Li} from the above equation, we get

$$C_{\text{Li}} = \frac{100 \rho_{\text{Li}} (\rho_{\text{Al}} - \rho_{\text{ave}})}{\rho_{\text{ave}} (\rho_{\text{Al}} - \rho_{\text{Li}})}$$

$$= \frac{(100)(0.534 \text{ g/cm}^3)(2.71 \text{ g/cm}^3 - 2.47 \text{ g/cm}^3)}{(2.47 \text{ g/cm}^3)(2.71 \text{ g/cm}^3 - 0.534 \text{ g/cm}^3)}$$

$$= 2.38 \text{ wt\%}$$

4.D2 This problem asks that we determine the concentration (in weight percent) of Cu that must be added to Pt so as to yield a unit cell edge length of 0.390 nm. To begin, it is necessary to employ Equation 3.5, and solve for the unit cell volume, V_C , as

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

where A_{ave} and ρ_{ave} are the atomic weight and density, respectively, of the Pt-Cu alloy. Inasmuch as both of these materials have the FCC crystal structure, which has cubic symmetry, V_C is just the cube of the unit cell length, *a*. That is

$$V_C = a^3 = (0.390 \text{ nm})^3$$

(3.90 × 10⁻⁸ cm)³ = 5.932 × 10⁻²³ cm³

It is now necessary to construct expressions for A_{ave} and ρ_{ave} in terms of the concentration of vanadium, C_{Cu} , using Equations 4.11a and 4.10a. For A_{ave} we have

$$A_{\text{ave}} = \frac{100}{\frac{C_{\text{Cu}}}{A_{\text{Cu}}} + \frac{(100 - C_{\text{Cu}})}{A_{\text{Pt}}}}$$

$$= \frac{100}{\frac{C_{\text{Cu}}}{63.55 \text{ g/mol}} + \frac{(100 - C_{\text{Cu}})}{195.08 \text{ g/mol}}}$$

whereas for ρ_{ave}

$$\rho_{\text{ave}} = \frac{100}{\frac{C_{\text{Cu}}}{\rho_{\text{Cu}}} + \frac{(100 - C_{\text{Cu}})}{\rho_{\text{Pt}}}}$$

| _ | 100 | | |
|---|-----------------------|-------------------------|--|
| _ | C _{Cu} | $(100 - C_{\rm Cu})$ | |
| | 8.94 g/cm^3 | 21.45 g/cm ³ | |

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Within the FCC unit cell there are 4 equivalent atoms, and thus, the value of n in Equation 3.5 is 4; hence, this expression may be written in terms of the concentration of Cu in weight percent as follows:

$$V_{C} = 5.932 \text{ x } 10^{-23} \text{ cm}^{3}$$

$$= \frac{nA_{\text{ave}}}{\rho_{\text{ave}}N_{\text{A}}}$$

$$= \frac{(4 \text{ atoms/unit cell}) \left[\frac{100}{\frac{C_{\text{Cu}}}{63.55 \text{ g/mol}} + \frac{(100 - C_{\text{Cu}})}{195.08 \text{ g/mol}}} \right]}{\left[\frac{100}{\frac{C_{\text{Cu}}}{8.94 \text{ g/cm}^{3}} + \frac{(100 - C_{\text{Cu}})}{21.45 \text{ g/cm}^{3}}} \right]} (6.023 \times 10^{23} \text{ atoms/mol})$$

And solving this expression for C_{Cu} leads to $C_{Cu} = 2.825$ wt%.