

Homework #4

Due: Feb 19, 2008

1. (a) The equilibrium number of vacancies N_v for a given quantity of material depends on and increases with temperature according to

$$N_v = N \exp\left(-\frac{Q_v}{kT}\right)$$

So, the fraction of vacant sites is:

$$\frac{N_v}{N} = \exp\left(-\frac{Q_v}{kT}\right)$$

Assume Q_v is 4eV, and therefore the fraction of vacant sites in Si at 1683K and 300K are respectively:

$$T=1683K, \quad \frac{N_v}{N} = \exp\left(-\frac{4eV}{(8.62 \times 10^{-5} eV/K)(1683K)}\right) = 1.06 \times 10^{-12}$$

$$T=300K, \quad \frac{N_v}{N} = \exp\left(-\frac{4eV}{(8.62 \times 10^{-5} eV/K)(300K)}\right) = 6.66 \times 10^{-68}$$

(b) The number of atomic sites per cubic meter for Si is according to:

$$\begin{aligned} N &= \frac{N_A \rho}{A_{Si}} \\ &= \frac{(6.02 \times 10^{23} \text{ atom/mol})(2.4 \text{ g/cm}^3)}{28.09 \text{ g/mol}} \\ &= 5.14 \times 10^{22} \text{ atom/cm}^3 \end{aligned}$$

Thus, the number of vacancies at 27°C (300K) is equal to

$$\begin{aligned} N_v &= N \exp\left(-\frac{Q_v}{kT}\right) \\ &= (5.14 \times 10^{22} \text{ atoms/cm}^3) \exp\left[-\frac{4eV}{(8.62 \times 10^{-5} eV/K)(300K)}\right] \\ &= 3.425 \times 10^{-45} \text{ vacancies/cm}^3 \end{aligned}$$

2. Assume that there is total 100g austenite with the concentration of 2.14 weight% carbon. So then the mass of C and Fe are 2.14g and 97.86g, respectively.

And the atom percent of C and Fe are:

$$C'_C = \frac{\frac{m_C}{A_C}}{\frac{m_C}{A_C} + \frac{m_{Fe}}{A_{Fe}}} = \frac{\frac{2.14g}{12.011g/mol}}{\frac{2.14g}{12.011g/mol} + \frac{97.86g}{55.847g/mol}} = 9.23mol\%$$

$$C'_{Fe} = \frac{\frac{m_{Fe}}{A_{Fe}}}{\frac{m_C}{A_C} + \frac{m_{Fe}}{A_{Fe}}} = \frac{\frac{97.86g}{55.847g/mol}}{\frac{2.14g}{12.011g/mol} + \frac{97.86g}{55.847g/mol}} = 90.77mol\%$$

3. (a) The mole percent of the four elements are: 17.3mol% Ni, 5.5mol% Zn, 2.2mol% Cu, 75mol% Au. Assume that there is totally 100mol white gold, and then the mass of the four elements are:

$$m_{Ni} = n_{Ni} \times A_{Ni} = 17.3mol \times 58.71g/mol = 1015.5g$$

$$m_{Zn} = n_{Zn} \times A_{Zn} = 5.5mol \times 65.4g/mol = 359.7g$$

$$m_{Cu} = n_{Cu} \times A_{Cu} = 2.2mol \times 63.5g/mol = 139.7g$$

$$m_{Au} = n_{Au} \times A_{Au} = 75mol \times 197g/mol = 14775g$$

$$m_{total} = 1015.5g + 359.7g + 139.7g + 14775g = 16289.9g$$

So the weight percent of the four elements are:

$$C_{Ni} = \frac{m_{Ni}}{m_{total}} \times 100 = \frac{1015.5g}{16289.9g} \times 100 = 6.2wt\%$$

$$C_{Zn} = \frac{m_{Zn}}{m_{total}} \times 100 = \frac{359.7g}{16289.9g} \times 100 = 2.2wt\%$$

$$C_{Cu} = \frac{m_{Cu}}{m_{total}} \times 100 = \frac{139.7g}{16289.9g} \times 100 = 0.8wt\%$$

$$C_{Au} = \frac{m_{Au}}{m_{total}} \times 100 = \frac{14775g}{16289.9g} \times 100 = 90.7wt\%$$

(b) The weight of Ni in a pendant that weights 7 gram is:

$$m_{Ni} = C_{Ni} \times m_{total} = 6.2wt\% \times 7g = 0.434g$$

4. The number of atoms per cubic centimeter of a) Cu and b) Au are:

$$\begin{aligned}
N_{Cu} &= \frac{N_A \rho_{Cu}}{A_{Cu}} \\
&= \frac{(6.02 \times 10^{23} \text{ atom/mol})(8.40 \text{ g/cm}^3)}{63.5 \text{ g/mol}} \\
&= 8.0 \times 10^{22} \text{ atom/cm}^3 \\
N_{Au} &= \frac{N_A \rho_{Au}}{A_{Au}} \\
&= \frac{(6.02 \times 10^{23} \text{ atom/mol})(19.32 \text{ g/cm}^3)}{196.9 \text{ g/mol}} \\
&= 5.9 \times 10^{22} \text{ atom/cm}^3
\end{aligned}$$

5. The alloy density can be expressed by

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

$$\text{or } \rho_{ave} = \frac{\frac{C_1' A_1}{\rho_1} + \frac{C_2' A_2}{\rho_2}}{\frac{C_1' A_1}{\rho_1} + \frac{C_2' A_2}{\rho_2}}$$

So the density of the composition in problem 3 is

$$\begin{aligned}
\rho_{ave} &= \frac{100}{\frac{C_1}{\rho_1} + \frac{C_2}{\rho_2} + \frac{C_3}{\rho_3} + \frac{C_4}{\rho_4}} \\
&= \frac{100}{\frac{6.2 \text{ wt}\%}{8.9 \text{ g/cm}^3} + \frac{2.2 \text{ wt}\%}{7.14 \text{ g/cm}^3} + \frac{0.8 \text{ wt}\%}{8.96 \text{ g/cm}^3} + \frac{90.7 \text{ wt}\%}{19.32 \text{ g/cm}^3}} \\
&= 17.28 \text{ g/cm}^3
\end{aligned}$$

5.9 (a) For Li^+ substituting for Ca^{2+} in CaO , oxygen vacancies would be created. For each Li^+ substituting for Ca^{2+} , one positive charge is removed; in order to maintain charge neutrality, a single negative charge may be removed. Negative charges are eliminated by creating oxygen vacancies, and for every two Li^+ ions added, a single oxygen vacancy is formed.

(b) For Cl^- substituting for O^{2-} in CaO , calcium vacancies would be created. For each Cl^- substituting for an O^{2-} , one negative charge is removed; in order to maintain charge neutrality, two Cl^- ions will lead to the formation of one calcium vacancy.

5.20 We are asked in this problem to determine the approximate density of a high-leaded brass that has a composition of 64.5 wt% Cu, 33.5 wt% Zn, and 2 wt% Pb. In order to solve this problem, Equation 5.10a is modified to take the following form:

$$\rho_{\text{ave}} = \frac{100}{\frac{C_{\text{Cu}}}{\rho_{\text{Cu}}} + \frac{C_{\text{Zn}}}{\rho_{\text{Zn}}} + \frac{C_{\text{Pb}}}{\rho_{\text{Pb}}}}$$

And, using the density values for Cu, Zn, and Pb appear inside the front cover of the text, the density is computed as follows:

$$\begin{aligned} \rho_{\text{ave}} &= \frac{100}{\frac{64.5 \text{ wt}\%}{8.94 \text{ g/cm}^3} + \frac{33.5 \text{ wt}\%}{7.13 \text{ g/cm}^3} + \frac{2 \text{ wt}\%}{11.35 \text{ g/cm}^3}} \\ &= 8.27 \text{ g/cm}^3 \end{aligned}$$

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

5.32 (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.