Homework 2 solutions

1. Vacant lattice sites in a metal crystal:

   Ratio :
   \[
   \left( \frac{n_v}{n_0} \right) = C e^{-\frac{E_v}{kT}}
   \]

   \(n_v/n_0\) : fraction of vacant aluminum lattice sites

   C: pre-exponential constant (from book) = 11.2

   \(E_v\): energy needed to create a vacancy = 0.76 eV

   k: Bolzman’s constant = 86.2(10)^{-6} eV/K

   T: Temperature

   T=550\degree C

   \[
   \left( \frac{n_v}{n_0} \right) = 11.2 e^{-\frac{0.76}{(86.2(10)^{-6})(823)}}
   \]

   \[
   \left( \frac{n_v}{n_0} \right) = 2.50(10)^{-4}
   \]

   T=23\degree C

   \[
   \left( \frac{n_v}{n_0} \right) = 11.2 e^{-\frac{0.76}{(86.2(10)^{-6})(298)}}
   \]

   \[
   \left( \frac{n_v}{n_0} \right) = 1.59(10)^{-12}
   \]

   The difference in the fractions is due to the increase in temperature…

   As the temperature increases towards the melting temperature, the fraction of
   vacancies increases significantly.
2.

\[ c_x = \left[1 - \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right)\right] \cdot (c_s - c_0) + c_0 \]

\[ D = D_0 e^{\frac{Q}{RT}} \]

\[ D_{C,1000°C} = 220(10)^{-6} e^{\frac{123(10)^3}{8.314(1273)}} \]

\[ D_{C,1000°C} = 2.17(10)^{-9} \frac{m^2}{s} \]

\[ c_s: \text{Determine} \quad x= 0 \text{ to } 1 \text{ mm} \]

\[ c_s = 0 \text{ (vacuum)} \quad t = 1 \text{ hour} = 3600 \text{ s} \]

\[ c_0 = 0.3 \text{ wt% C} \]

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Carbon Concentration Profile with in 1mm of the Carbon Free Surface

\[ y = -0.0035x^2 + 0.0624x - 0.0002 \]

\[ R^2 = 0.9998 \]
3.

a.) Self-diffusivity of Fe in $\alpha$-iron at 900°C [Fe diffusing in its own lattice, BCC ($\alpha$-iron), as an “substitutional” element.]

\[
D = D_0 e^{\frac{Q}{RT}} \quad D = 22(10)^{-6} e^{\frac{268(10)^3}{8.314*1173}}
\]

\[
D = 2.56(10)^{-17} \text{ m}^2/\text{s}
\]

b.) Self-diffusivity of Fe in $\gamma$-iron at 1000°C [Fe diffusing in its own lattice, FCC ($\gamma$-iron), as an “substitutional” element.]

\[
D = D_0 e^{\frac{Q}{RT}} \quad D = 200(10)^{-6} e^{\frac{240(10)^3}{8.314*1273}}
\]

\[
D = 2.84(10)^{-14} \text{ m}^2/\text{s}
\]

c.) Carbon diffusion in $\alpha$-iron at 900°C

\[
D = D_0 e^{\frac{Q}{RT}} \quad D = 20(10)^{-6} e^{\frac{142(10)^3}{8.314*1173}}
\]

\[
D = 9.49(10)^{-12} \text{ m}^2/\text{s}
\]

d.) Carbon diffusion in $\gamma$-iron at 1000°C

\[
D = D_0 e^{\frac{Q}{RT}} \quad D = 220(10)^{-6} e^{\frac{122(10)^3}{8.314*1273}}
\]

\[
D = 2.17(10)^{-9} \text{ m}^2/\text{s}
\]
e.) Interstitial diffusion (c,d) is a quicker motion than substitutional diffusion (a,b) because the activation energy levels are lower. In substitutional diffusion, the formation of a vacancy is required, whereas in interstitial diffusion, it is not.

   2. The same crystal structure.
   3. Less than 0.4 difference in electronegativity.
   4. The same valence.

Al-Mg system: violates rules 2 and 4

Al is FCC and +3 valence
Mg is HCP and +2 valence
(Approximately 11% difference in radii and 0.3 difference in electronegativity)

Area of interest is the Mg side (the δ phase)
Al-Cu system: violates rules 3 and 4

Al has 1.5 electronegativity and +3 valence

Cu has 1.9 electronegativity and +2 valence

(Approximately 13% difference in radii and both are FCC)

Area of interest is the Cu side (the $\alpha$ phase)
5. \( F = C - P + 2 \)

a.) \( C = 1 \)

\[ P = 3 (\alpha, \beta, \text{gas}) \text{ or } (\gamma, \text{liq, gas}) \]

\[ F = 1 - 3 + 2 = 0 \]

At the triple points, there are 0 degrees of freedom. The triple points are set, i.e. there can be no variation in temperature or pressure.

b.) \( C = 1 \)

\[ P = 2 (\text{gas, liq}) \]

\[ F = 1 - 2 + 2 = 1 \]

Along the liquid-gas condensation line, there is 1 degree of freedom. Only one variable, \( P \) or \( T \), can be varied, but not both. If \( P \) is varied, then \( T \) is fixed and vice versa.
6. 500g of 30% Pb and 70% Sn cooled from 300°C

   a. 190°C
   Composition of each phase: Liquid ~ 69 w% Sn / 31 w% Pb
      Proeutectic Beta ~ 98 w% Sn / 2 w% Pb

      Grams of Proeutectic Beta: \[
      \left( \frac{70 - 69}{98 - 69} \right) \cdot 500 = 17.3 \text{ g of Proeutectic Beta.}
      \]

      Grams of Liquid: \[
      \left( \frac{98 - 70}{98 - 69} \right) \cdot 500 = 482.7 \text{ g of Liquid.}
      \]

   b. Just above 183°C
   Composition of each phase: Liquid ~ 61.9 w% Sn / 38.1 w% Pb
      Proeutectic Beta ~ 97.5 w% Sn / 2.5 w% Pb

      Grams of Proeutectic Beta: \[
      \left( \frac{70 - 61.9}{97.5 - 61.9} \right) \cdot 500 = 113.8 \text{ g of Proeutectic Beta.}
      \]

      Grams of Liquid: \[
      \left( \frac{97.5 - 70}{97.5 - 61.9} \right) \cdot 500 = 382.2 \text{ g of Liquid.}
      \]

   c. Just below 183°C
   Composition of each phase: Alpha ~ 19 w% Sn / 81 w% Pb
      Beta ~ 97.5 w% Sn / 2.5 w% Pb

      Grams of Alpha: \[
      \left( \frac{97.5 - 70}{97.5 - 19} \right) \cdot 500 = 175.2 \text{ g of Alpha.}
      \]

      Grams of Beta: \[
      \left( \frac{70 - 19}{97.5 - 19} \right) \cdot 500 = 324.8 \text{ g of Beta.}
      \]

   d. At Room Temperature (Assume 25°C)
   Composition of each phase: Alpha ~ 1 w% Sn / 99 w% Pb
      Tin ~ 100 w% Sn

      Grams of Alpha: \[
      \left( \frac{100 - 70}{100 - 1} \right) \cdot 500 = 151.5 \text{ g of Alpha.}
      \]

      Grams of Beta: \[
      \left( \frac{70 - 1}{100 - 1} \right) \cdot 500 = 348.5 \text{ g of Beta.}
      \]
Pb-Sn phase diagram