HW 5

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E45

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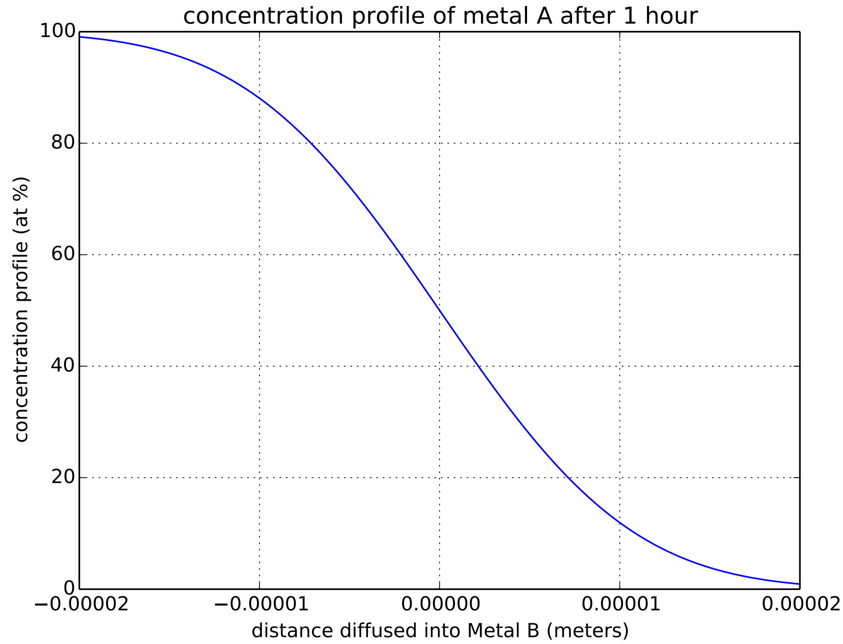
Problem 5.10. Carburization was described in Example 5.3. The decarburization of a steel can also be described by using the error function. Starting with Equation 5.11 and taking $c_s = 0$, derive an expression to describe the concentration profile of carbon as it diffuses out of a steel with initial concentration, c_0. (This situation can be produced by placing the steel in a vacuum at elevated temperature.)

$$\begin{aligned}
\frac{c_x - c_0}{c_s - c_0} &= 1 - \operatorname{erf}(\frac{x}{2\sqrt{Dt}}), \text{take } c_s = 0 \\
\frac{c_x - c_0}{0 - c_0} &= 1 - \operatorname{erf}(\frac{x}{2\sqrt{Dt}}) \\
\frac{c_x - c_0}{-c_0} &= 1 - \operatorname{erf}(\frac{x}{2\sqrt{Dt}}) \\
\frac{c_0 - c_x}{c_0} &= 1 - \operatorname{erf}(\frac{x}{2\sqrt{Dt}}) \\
1 - \frac{c_x}{c_0} &= 1 - \operatorname{erf}(\frac{x}{2\sqrt{Dt}}) \\
-\frac{c_x}{c_0} &= -\operatorname{erf}(\frac{x}{2\sqrt{Dt}}) \\
\frac{c_x}{c_0} &= \operatorname{erf}(\frac{x}{2\sqrt{Dt}}) \ <- \text{answer}
\end{aligned}$$

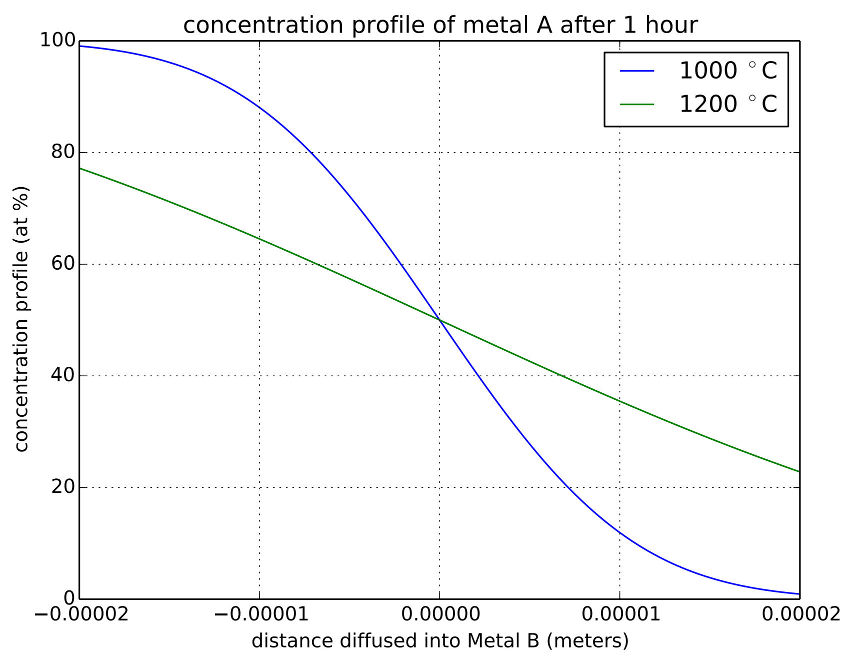
Problem 5.12. A diffusion couple is formed when two different materials are allowed to interdiffuse at an elevated temperature (see Figure 5.8). For a block of pure metal A adjacent to a block of pure metal B, the concentration profile of A (in at%) after interdiffusion is given by

$$c_x = 50[1 - \operatorname{erf}(\frac{x}{2\sqrt{Dt}})] \tag{1}$$

where x is measured from the original interface. For a diffusion couple with $D = 10^{-14}\, m^2/s$, plot the concentration profile of metal A over a range of 20 μm on either side of the original interface (x = 0) after a time of 1 hour. [Note that erf (-z) = –erf (z).]



Problem 5.14. Using the results of Problem **5.12** and assuming that profile occurred at a temperature of 1,000°C, superimpose the concentration profile of metal A for the same diffusion couple for 1 hour but heated at 1,200°C at which D = $10^{-13}\, m^2/s$.



Problem 5.24. Diffusion length, λ, is a popular term in characterizing the production of semiconductors by the controlled diffusion of impurities into a high-purity material. The

value of λ is taken as $2\sqrt{Dt}$, where λ represents the extent of diffusion for an impurity with a diffusion coefficient, D, over a period of time, t. Calculate the diffusion length of B in Ge for a total diffusion time of 30 minutes at a temperature of **(a)** 800°C and **(b)** 900°C.

Using the data from Table 5.3 on page 139 of Shackelford [1] we see that for B Ge $D_0 = 1.1 \times 10^3 m^2/s$ and $Q = 439kJ/mol$.

$$D = D_0 \mathrm{e}^{\frac{-Q}{RT}} \tag{2}$$

where D_0 is the preexponential constant, Q is the activation energy, R is the gas constant, and T is temperature

(a)

$$\lambda = \sqrt{Dt} = \sqrt{D_0 \mathrm{e}^{\frac{-Q}{RT}} t} = \sqrt{1.1 \times 10^3 m^2/s \, \mathrm{e}^{\frac{-439000J}{(8.314)(800+273.15)K}} * 1800s} = 29.1\,\mathrm{nm}$$

(b)

$$\lambda = \sqrt{Dt} = \sqrt{D_0 \mathrm{e}^{\frac{-Q}{RT}} t} = \sqrt{1.1 \times 10^3 m^2/s \, \mathrm{e}^{\frac{-439000J}{(8.314)(900+273.15)K}} * 1800s} = 238\,\mathrm{nm}$$

Problem 5.29. The endpoints of the Arrhenius plot of $D_{\text{grain boundary}}$ in Figure 5.18 are $D_{\text{grain boundary}} = 3.2 \times 10^{-12} m^2/s$ at a temperature of $457°C$ and $D_{\text{grain boundary}} = 1.0 \times 10^{-10} m^2/s$ at a temperature of $689°C$. Using these data, calculate the activation energy for grain boundary diffusion is silver.

$$D_2 = D_0 \mathrm{e}^{\frac{-Q}{RT_2}} \tag{3}$$

$$D_1 = D_0 \mathrm{e}^{\frac{-Q}{RT_1}} \tag{4}$$

Where $D_2 = 3.2 \times 10^{-12} m^2/s$, $D_1 = 1.0 \times 10^{-10} m^2/s$, $T_2 = 730.15K$, and $T_1 = 962.15$. Divide equation 3 by equation 4

$$\frac{D_2 = D_0 \mathrm{e}^{\frac{-Q}{RT_2}}}{D_1 = D_0 \mathrm{e}^{\frac{-Q}{RT_1}}} \Rightarrow \frac{D_2}{D_1} = \frac{\mathrm{e}^{\frac{Q}{RT_1}}}{\mathrm{e}^{\frac{Q}{RT_2}}} \Rightarrow \frac{D_2}{D_1} = \mathrm{e}^{\frac{Q}{R}(\frac{1}{T_1} - \frac{1}{T_2})} \Rightarrow \ln(\frac{D_2}{D_1}) = \ln(\mathrm{e}^{\frac{Q}{R}(\frac{1}{T_1} - \frac{1}{T_2})})$$

$$\ln(\frac{D_2}{D_1}) = \frac{Q}{R}(\frac{1}{T_1} - \frac{1}{T_2}) \Rightarrow Q = \frac{RT_2T_1\ln(\frac{D_2}{D_1})}{T_1 - T_2} = \frac{8.315 * 730.15K * 962.15\ln(\frac{3.2\times10^{-12}}{1.0\times10^{-10}})}{962.15 - 730.15}$$

$$Q = -86664.74\,\text{Joules/mole} = -86.7\,\text{kJ/mole}$$

1 References

1. James F. Shackelford, Introduction to Materials Science for Engineers, Seventh Edition, Pearson Higher Education, Inc., Upper Saddle River, New Jersey (2009).