Diffusion Mechanisms

5.3 (a) With vacancy diffusion, atomic motion is from one lattice site to an adjacent vacancy. Self-diffusion and the diffusion of substitutional impurities proceed via this mechanism. On the other hand, atomic motion is from interstitial site to adjacent interstitial site for the interstitial diffusion mechanism.

(b) Interstitial diffusion is normally more rapid than vacancy diffusion because: (1) interstitial atoms, being smaller, are more mobile; and (2) the probability of an empty adjacent interstitial site is greater than for a vacancy adjacent to a host (or substitutional impurity) atom.

Steady-State Diffusion

5.4 Steady-state diffusion is the situation wherein the rate of diffusion into a given system is just equal to the rate of diffusion out, such that there is no net accumulation or depletion of diffusing species--i.e., the diffusion flux is independent of time.

5.6 This problem calls for the mass of hydrogen, per hour, that diffuses through a Pd sheet. It first becomes necessary to employ both Equations 5.1a and 5.3. Combining these expressions and solving for the mass yields

$$M = JAt = -DAt\frac{\Delta C}{\Delta x}$$

$$= -(1.7 \times 10^{-8}\ \text{m}^2/\text{s})(0.25\ \text{m}^2)(3600\ \text{s/h})\left[\frac{0.4 - 2.0\ \text{kg/m}^3}{6 \times 10^{-3}\ \text{m}}\right]$$

$$= 4.1 \times 10^{-3}\ \text{kg/h}$$

5.11 We are asked to compute the carburizing (i.e., diffusion) time required for a specific nonsteady-state diffusion situation. It is first necessary to use Equation 5.5:

$$\frac{C_x - C_0}{C_s - C_0} = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

wherein, C_x = 0.30, C_0 = 0.10, C_s = 0.90, and x = 4 mm = 4 x 10^{-3} m. Thus,

$$\frac{C_x - C_0}{C_s - C_0} = \frac{0.30 - 0.10}{0.90 - 0.10} = 0.2500 = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

or

$$\operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) = 1 - 0.2500 = 0.7500$$

By linear interpolation using data from Table 5.1

z	erf(z)
0.80	0.7421
z	0.7500
0.85	0.7707

$$\frac{z - 0.800}{0.850 - 0.800} = \frac{0.7500 - 0.7421}{0.7707 - 0.7421}$$

From which

$$z = 0.814 = \frac{x}{2\sqrt{Dt}}$$

Now, from Table 5.2, at 1100°C (1373 K)

$$D = \left(2.3 \times 10^{-5}\ \text{m}^2/\text{s}\right) \exp\left[-\frac{148{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(1373\ \text{K})}\right]$$

$$= 5.35 \times 10^{-11}\ \text{m}^2/\text{s}$$

Thus,

$$0.814 = \frac{4 \times 10^{-3} \text{ m}}{(2)\sqrt{(5.35 \times 10^{-11} \text{ m}^2/\text{s})(t)}}$$

Solving for *t* yields

$$t = 1.13 \text{ x } 10^5 \text{ s} = 31.3 \text{ h}$$

5.12 This problem asks that we determine the position at which the carbon concentration is 0.25 wt% after a 10-h heat treatment at 1325 K when C_0 = 0.55 wt% C. From Equation 5.5

$$\frac{C_x - C_0}{C_s - C_0} = \frac{0.25 - 0.55}{0 - 0.55} = 0.5455 = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

Thus,

$$\operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) = 0.4545$$

Using data in Table 5.1 and linear interpolation

z	erf (z)
0.40	0.4284
z	0.4545
0.45	0.4755

$$\frac{z - 0.40}{0.45 - 0.40} = \frac{0.4545 - 0.4284}{0.4755 - 0.4284}$$

And,

$$z = 0.4277$$

Which means that

$$\frac{x}{2\sqrt{Dt}} = 0.4277$$

And, finally

$$x = 2(0.4277)\sqrt{Dt} = (0.8554)\sqrt{(4.3 \times 10^{-11}\ \text{m}^2/\text{s})(3.6 \times 10^4\ \text{s})}$$

$$= 1.06 \text{ x } 10^{-3} \text{ m} = 1.06 \text{ mm}$$

Note: this problem may also be solved using the "Diffusion" module in the *VMSE* software. Open the "Diffusion" module, click on the "Diffusion Design" submodule, and then do the following:

1. Enter the given data in left-hand window that appears. In the window below the label “D Value” enter the value of the diffusion coefficient—viz. “4.3e-11”.

2. In the window just below the label “Initial, C0” enter the initial concentration—viz. “0.55”.

3. In the window the lies below “Surface, Cs” enter the surface concentration—viz. “0”.

4. Then in the “Diffusion Time t” window enter the time in seconds; in 10 h there are (60 s/min)(60 min/h)(10 h) = 36,000 s—so enter the value “3.6e4”.

5. Next, at the bottom of this window click on the button labeled “Add curve”.

6. On the right portion of the screen will appear a concentration profile for this particular diffusion situation. A diamond-shaped cursor will appear at the upper left-hand corner of the resulting curve. Click and drag this cursor down the curve to the point at which the number below “Concentration:” reads “0.25 wt%”. Then read the value under the “Distance:”. For this problem, this value (the solution to the problem) is 1.05 mm.

5.13 This problem asks us to compute the nitrogen concentration (C_x) at the 2 mm position after a 25 h diffusion time, when diffusion is nonsteady-state. From Equation 5.5

$$\frac{C_x - C_0}{C_s - C_0} = \frac{C_x - 0}{0.2 - 0} = 1 - \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

$$= 1 - \text{erf}\left[\frac{2 \times 10^{-3}\text{ m}}{(2)\sqrt{(1.9 \times 10^{-11}\text{ m}^2/\text{s})(25\text{ h})(3600\text{ s/h})}}\right]$$

$$= 1 - \text{erf}\ (0.765)$$

Using data in Table 5.1 and linear interpolation

<u>*z*</u>	<u>erf (*z*)</u>
0.750	0.7112
0.765	*y*
0.800	0.7421

$$\frac{0.765 - 0.750}{0.800 - 0.750} = \frac{y - 0.7112}{0.7421 - 0.7112}$$

from which

$$y = \text{erf}\ (0.765) = 0.7205$$

Thus,

$$\frac{C_x - 0}{0.2 - 0} = 1.0 - 0.7205$$

This expression gives

$$C_x = 0.056\text{ wt\% N}$$

Note: this problem may also be solved using the “Diffusion” module in the *VMSE* software. Open the “Diffusion” module, click on the “Diffusion Design” submodule, and then do the following:

1. Enter the given data in left-hand window that appears. In the window below the label "D Value" enter the value of the diffusion coefficient—viz. "1.9e-11".

2. In the window just below the label "Initial, C0" enter the initial concentration—viz. "0".

3. In the window the lies below "Surface, Cs" enter the surface concentration—viz. "0.2".

4. Then in the "Diffusion Time t" window enter the time in seconds; in 25 h there are (60 s/min)(60 min/h)(25 h) = 90,000 s—so enter the value "9e4".

5. Next, at the bottom of this window click on the button labeled "Add curve".

6. On the right portion of the screen will appear a concentration profile for this particular diffusion situation. A diamond-shaped cursor will appear at the upper left-hand corner of the resulting curve. Click and drag this cursor down the curve to the point at which the number below "Distance:" reads "2.00 mm". Then read the value under the "Concentration:". For this problem, this value (the solution to the problem) is 0.06 wt%.

5.15 This problem calls for an estimate of the time necessary to achieve a carbon concentration of 0.35 wt% at a point 6.0 mm from the surface. From Equation 5.6b,

$$\frac{x^2}{Dt} = \text{constant}$$

But since the temperature is constant, so also is *D* constant, and

$$\frac{x^2}{t} = \text{constant}$$

or

$$\frac{x_1^2}{t_1} = \frac{x_2^2}{t_2}$$

Thus,

$$\frac{(2.0 \text{ mm})^2}{15 \text{ h}} = \frac{(6.0 \text{ mm})^2}{t_2}$$

from which

$$t_2 = 135 \text{ h}$$

5.17 This problem asks us to compute the magnitude of *D* for the diffusion of Mg in Al at 400°C (673 K). Incorporating the appropriate data from Table 5.2 into Equation 5.8 leads to

$$D = (1.2 \times 10^{-4} \text{ m}^2/\text{s}) \exp\left[-\frac{131{,}000 \text{ J/mol}}{(8.31 \text{ J/mol-K})(673 \text{ K})}\right]$$

$$= 8.1 \times 10^{-15} \text{ m}^2/\text{s}$$

Note: this problem may also be solved using the "Diffusion" module in the *VMSE* software. Open the "Diffusion" module, click on the "D vs 1/T Plot" submodule, and then do the following:

1. In the left-hand window that appears, click on the "Mg-Al" pair under the "Diffusing Species"-"Host Metal" headings.

2. Next, at the bottom of this window, click the "Add Curve" button.

3. A log D versus 1/T plot then appears, with a line for the temperature dependence of the diffusion coefficient for Mg in Al. At the top of this curve is a diamond-shaped cursor. Click-and-drag this cursor down the line to the point at which the entry under the "Temperature (T):" label reads 673 K (inasmuch as this is the Kelvin equivalent of 400ºC). Finally, the diffusion coefficient value at this temperature is given under the label "Diff Coeff (D):". For this problem, the value is 7.8 x 10^{-15} m^2/s.