

재료공학 원리 Homework

5 장 Diffusion 예제문제

$$\frac{x}{2\sqrt{Dt}} = z \Rightarrow t = \left(\frac{x}{2z}\right)^2 \cdot \frac{1}{D}$$

$$\therefore t = \left(\frac{5 \times 10^{-4} \text{ m}}{2 \times 0.3993}\right)^2 \frac{1}{1.6 \times 10^{-11} \text{ m}^2/\text{s}}$$

$$= 25775 \text{ s} = \underline{7.2 \text{ h}}$$

1.

EXAMPLE PROBLEM 7.1

Diffusion Flux Computation

A plate of iron is exposed to a carburizing (carbon-rich) atmosphere on one side and a decarburizing (carbon-deficient) atmosphere on the other side at 700°C. If a condition of steady state is achieved, calculate the diffusion flux of carbon through the plate if the concentrations of carbon at positions of 5 and 10 mm (5×10^{-3} and 10^{-2} m) beneath the carburizing surface are 1.2 and 0.8 kg/m³, respectively. Assume a diffusion coefficient of 3×10^{-11} m²/s at this temperature.

$$J = -D \frac{dc}{dx}$$

$$= -3 \times 10^{-11} \text{ m}^2/\text{s} \cdot \frac{(0.9 - 1.2) \text{ kg/m}^3}{(10^{-2} - 5 \times 10^{-3}) \text{ m}}$$

$$= \underline{2.4 \times 10^{-9} \text{ kg} \cdot \text{m}^{-2} \cdot \text{s}^{-1}}$$

2.

EXAMPLE PROBLEM 7.2

Nonsteady-State Diffusion Time Computation I

For some applications, it is necessary to harden the surface of a steel (or iron-carbon alloy) above that of its interior. One way this may be accomplished is by increasing the surface concentration of carbon in a process termed **carburizing**: the steel piece is exposed, at an elevated temperature, to an atmosphere rich in a hydrocarbon gas, such as methane (CH₄).

Consider one such alloy that initially has a uniform carbon concentration of 0.25 wt% and is to be treated at 950°C. If the concentration of carbon at the surface is suddenly brought to and maintained at 1.20 wt%, how long will it take to achieve a carbon content of 0.80 wt% at a position 0.5 mm below the surface? The diffusion coefficient for carbon in iron at this temperature is 1.6×10^{-11} m²/s; assume that the steel piece is semi-infinite.

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

$$x = 0.5 \text{ mm} = 5 \times 10^{-4} \text{ m} \quad D = 1.6 \times 10^{-11} \text{ m}^2/\text{s}$$

$$C_0 = 0.25 \text{ wt\%} \quad C_x = 0.80 \text{ wt\%}$$

$$C_s = 1.20 \text{ wt\%}$$

$$\text{erf}\left(\frac{x}{2\sqrt{Dt}}\right) = 1 - \frac{C_x - C_0}{C_s - C_0} = 0.4211$$

$$\text{erf}(0.35) = 0.3794, \quad \text{erf}(0.40) = 0.4284$$

$$\frac{z - 0.35}{0.40 - 0.35} = \frac{0.4211 - 0.3794}{0.4284 - 0.3794} \quad \therefore z = 0.3993$$

3.

EXAMPLE PROBLEM 7.3

Nonsteady-State Diffusion Time Computation II

The diffusion coefficients for copper in aluminum at 500°C and 600°C are 4.8×10^{-14} and 5.3×10^{-13} m²/s, respectively. Determine the approximate time at 500°C that will produce the same diffusion result (in terms of concentration of Cu at some specific point in Al) as a 10-h heat treatment at 600°C.

$$D_{500^\circ\text{C}} = 4.8 \times 10^{-14} \text{ m}^2/\text{s}, \quad D_{600^\circ\text{C}} = 5.3 \times 10^{-13} \text{ m}^2/\text{s}$$

$$\frac{C_x - C_0}{C_s - C_0} = 1 - \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \text{ 이어서, 같은 } (x, C_s, C_0 \text{ 이대개 같은 값을}$$

가져오야 한다. 따라서 $t_{500^\circ\text{C}}$ 생성한다

$$D_{500^\circ\text{C}} t_{500^\circ\text{C}} = D_{600^\circ\text{C}} t_{600^\circ\text{C}}$$

$$t_{500^\circ\text{C}} = (5.3 \times 10^{-13} \text{ m}^2/\text{s} \times 1.6 \times 10^4 \text{ s}) / (4.8 \times 10^{-14} \text{ m}^2/\text{s})$$

$$= 3.975 \times 10^5 \text{ s} = \underline{110.4 \text{ h}}$$

4.

EXAMPLE PROBLEM 7.4

Diffusion Coefficient Determination

Using the data in Table 7.2, compute the diffusion coefficient for magnesium in aluminum at 550°C.

Table 7.2

A Tabulation of Diffusion Data

Diffusing Species	Host Metal	D_0 (m ² /s)	Q_d (J/mol)
Interstitial Diffusion			
C ^b	Fe (α or BCC) ^a	1.1×10^{-6}	87,400
C ^c	Fe (γ or FCC) ^a	2.3×10^{-5}	148,000
N ^b	Fe (α or BCC) ^a	5.0×10^{-7}	77,000
N ^c	Fe (γ or FCC) ^a	9.1×10^{-5}	168,000
Self-Diffusion			
Fe ^c	Fe (α or BCC) ^a	2.8×10^{-4}	251,000
Fe ^c	Fe (γ or FCC) ^a	5.0×10^{-5}	284,000
Cu ^d	Cu (FCC)	2.5×10^{-5}	200,000
Al ^f	Al (FCC)	2.3×10^{-4}	144,000
Mg ^g	Mg (HCP)	1.5×10^{-4}	136,000
Zn ^h	Zn (HCP)	1.5×10^{-5}	94,000
Mo ⁱ	Mo (BCC)	1.8×10^{-4}	461,000
Ni ^j	Ni (FCC)	1.9×10^{-4}	285,000
Interdiffusion (Vacancy)			
Zn ^h	Cu (FCC)	2.4×10^{-5}	189,000
Cu ^h	Zn (HCP)	2.1×10^{-4}	124,000
Cu ^h	Al (FCC)	6.5×10^{-5}	136,000
Mg ^g	Al (FCC)	1.2×10^{-4}	130,000
Cu ^h	Ni (FCC)	2.7×10^{-5}	256,000
Ni ^j	Cu (FCC)	1.9×10^{-4}	230,000

$$D = D_0 \exp\left(-\frac{Q_d}{RT}\right)$$

$$= 1.2 \times 10^{-4} \text{ m}^2/\text{s} \cdot \exp\left(-\frac{1.3 \times 10^5 \text{ J/mol}}{8.31 \text{ J/mol} \cdot \text{K} \cdot (550 + 273) \text{ K}}\right)$$

$$= \underline{6.7 \times 10^{-11} \text{ m}^2/\text{s}}$$

5.

EXAMPLE PROBLEM 7.5

Diffusion Coefficient Activation Energy and Preexponential Calculations

Figure 7.8 shows a plot of the logarithm (to the base 10) of the diffusion coefficient versus reciprocal of absolute temperature for the diffusion of copper in gold. Determine values for the activation energy and the preexponential.

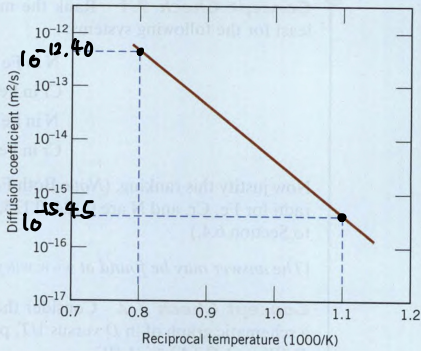


Figure 7.8 Plot of the logarithm of the diffusion coefficient versus the reciprocal of absolute temperature for the diffusion of copper in gold.

$$D = D_0 \exp\left(-\frac{Q_d}{RT}\right)$$

$$\ln D = \ln D_0 - \frac{Q_d}{R} \cdot \frac{1}{T}$$

$$\ln D_2 / D_1 = -\frac{Q_d}{R} \left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

$$D_1 = 10^{-12.40} \text{ m}^2/\text{s}, D_2 = 10^{-15.45} \text{ m}^2/\text{s}$$

$$\frac{1}{T_1} = 0.9 \times 10^{-3} \text{ K}^{-1}, \frac{1}{T_2} = 1.1 \times 10^{-3} \text{ K}^{-1}$$

$$\begin{aligned} Q_d &= \left(\frac{\ln D_2 - \ln D_1}{1/T_2 - 1/T_1} \right) \cdot (-R) \\ &= \frac{(-15.45 + 12.40) \cdot \ln 10}{(1.1 - 0.9) \times 10^{-3} \text{ K}^{-1}} \cdot (-8.31 \text{ J/mol}\cdot\text{K}) \\ &= \underline{194 \text{ kJ/mol}} \end{aligned}$$

$$\begin{aligned} D_0 &= D_1 / \exp\left(-\frac{Q_d}{R} \cdot \frac{1}{T_1}\right) \\ &= 10^{-12.40} \text{ m}^2/\text{s} / \exp\left(-\frac{194 \cdot 10^3 \text{ J/mol}}{8.31 \text{ J/mol}\cdot\text{K}} \cdot 0.9 \times 10^{-3} \text{ K}^{-1}\right) \\ &= \underline{5.14 \times 10^{-5} \text{ m}^2/\text{s}} \end{aligned}$$

6.

EXAMPLE PROBLEM 7.6

Diffusion of Boron into Silicon

Boron atoms are to be diffused into a silicon wafer using both predeposition and drive-in heat treatments; the background concentration of B in this silicon material is known to be 1×10^{20} atoms/m³. The predeposition treatment is to be conducted at 900°C for 30 min; the surface concentration of B is to be maintained at a constant level of 3×10^{26} atoms/m³. Drive-in diffusion will be carried out at 1100°C for a period of 2 h. For the diffusion coefficient of B in Si, values of Q_d and D_0 are 3.87 eV/atom and 2.4×10^{-3} m²/s, respectively.

- (a) Calculate the value of Q_0 .
- (b) Determine the value of x_j for the drive-in diffusion treatment.
- (c) Also for the drive-in treatment, compute the concentration of B atoms at a position 1 μm below the surface of the silicon wafer.

$$(a) Q_0 = 2C_s \sqrt{\frac{D_0 t_p}{\pi}}$$

$$C_s = 3 \times 10^{26} \text{ atoms/m}^3$$

$$t_p = 30 \text{ min} = 1800 \text{ s}$$

$$D_p = D_0 \exp\left(-\frac{Q_d}{RT}\right)$$

$$= 2.4 \times 10^{-3} \text{ m}^2/\text{s} \cdot \exp\left(-\frac{3.87 \text{ eV/atom} \cdot \frac{6.02 \times 10^{23} \text{ atoms}}{1 \text{ mol}} \cdot \frac{1.602 \times 10^{-19} \text{ J}}{1 \text{ eV}}}{8.31 \text{ J/mol}\cdot\text{K} \cdot (900 + 273) \text{ K}}\right)$$

$$= 5.72 \times 10^{-20} \text{ m}^2/\text{s}$$

$$\therefore Q_0 = 2 \cdot 3 \times 10^{26} \text{ atoms/m}^3 \cdot \sqrt{5.72 \times 10^{-20} \text{ m}^2/\text{s} \cdot 1800 \text{ s}} / \sqrt{\pi}$$

$$= \underline{3.44 \times 10^{18} \text{ atoms/m}^2}$$

$$(b) x_j = \sqrt{4D_d t_d \ln\left(\frac{Q_0}{C_0 \sqrt{\pi D_d t_d}}\right)}$$

$$t_d = 2 \text{ h} = 7200 \text{ s}$$

$$Q_0 = 3.44 \times 10^{18} \text{ atoms/m}^2$$

$$C_0 = 1 \times 10^{20} \text{ atoms/m}^3$$

$$D_d = D_0 \exp\left(-\frac{Q_d}{RT}\right)$$

$$= 2.4 \times 10^{-3} \text{ m}^2/\text{s} \cdot \exp\left(-\frac{3.87 \text{ eV/atom} \cdot \frac{6.02 \times 10^{23} \text{ atoms}}{1 \text{ mol}} \cdot \frac{1.602 \times 10^{-19} \text{ J}}{1 \text{ eV}}}{8.31 \text{ J/mol}\cdot\text{K} \cdot (1100 + 273) \text{ K}}\right)$$

$$= 1.51 \times 10^{-19} \text{ m}^2/\text{s}$$

$$\therefore x_j = \sqrt{4 \cdot 1.51 \times 10^{-19} \text{ m}^2/\text{s} \cdot 7200 \text{ s} \cdot \ln\left(\frac{3.44 \times 10^{18} \text{ atoms/m}^2}{1 \cdot 10^{20} \text{ atoms/m}^3 \cdot \sqrt{\pi \cdot 1.51 \times 10^{-19} \text{ m}^2/\text{s} \cdot 7200 \text{ s}}}\right)}$$

$$= \underline{2.1 \mu\text{m}}$$

$$(c) C(x, t) = \frac{Q_0}{\sqrt{\pi D_d t}} \exp\left(-\frac{x^2}{4D_d t}\right) \quad x = 1 \mu\text{m}$$

$$= \frac{3.44 \times 10^{18} \text{ atoms/m}^2}{\sqrt{\pi \cdot 1.51 \times 10^{-19} \text{ m}^2/\text{s} \cdot 7200 \text{ s}}} \cdot \exp\left(-\frac{(1 \times 10^{-6} \text{ m})^2}{4 \cdot 1.51 \times 10^{-19} \text{ m}^2/\text{s} \cdot 7200 \text{ s}}\right)$$

$$= \underline{5.90 \times 10^{14} \text{ atoms/m}^3}$$

7.

EXAMPLE PROBLEM 7.7

Computations of Diffusion Flux of Carbon Dioxide through a Plastic Beverage Container and Beverage Shelf Life

The clear plastic bottles used for carbonated beverages (sometimes also called *soda*, *pop*, or *soda pop*) are made from poly(ethylene terephthalate) (PET). The “fizz” in pop results from dissolved carbon dioxide (CO₂); because PET is permeable to CO₂, pop stored in PET bottles will eventually go “flat” (i.e., lose its fizz). A 0.6 L bottle of pop has a CO₂ pressure of about 400 kPa inside the bottle, and the CO₂ pressure outside the bottle is 0.4 kPa.

- (a) Assuming conditions of steady state, calculate the diffusion flux of CO₂ through the wall of the bottle.
- (b) If the bottle must lose 750 (cm³ STP) of CO₂ before the pop tastes flat, what is the shelf life for a bottle of pop?

Note: Assume that each bottle has a surface area of 500 cm² and a wall thickness of 0.05 cm.

Table 7.4
Permeability Coefficient P_M at 25°C for Oxygen, Nitrogen, Carbon Dioxide, and Water Vapor in a Variety of Polymers

Polymer	Acronym	P _M [× 10 ⁻¹³ (cm ³ STP)(cm)/(cm ² ·s·Pa)]			
		O ₂	N ₂	CO ₂	H ₂ O
Polyethylene (low density)	LDPE	2.2	0.73	9.5	68
Polyethylene (high density)	HDPE	0.30	0.11	0.27	9.0
Polypropylene	PP	1.2	0.22	5.4	38
Poly(vinyl chloride)	PVC	0.034	0.0089	0.012	206
Polystyrene	PS	2.0	0.59	7.9	840
Poly(vinylidene chloride)	PVDC	0.0025	0.00044	0.015	7.0
Poly(ethylene terephthalate)	PET	0.044	0.011	0.23	—
Poly(ethyl methacrylate)	PEMA	0.89	0.17	3.8	2380

Source: Adapted from J. Brandrup, E. H. Immergut, E. A. Grulke, A. Abe, and D. R. Bloch (Editors). *Polymer Handbook*, 4th edition. Copyright © 1999 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.

Table 7.4 presents the permeability coefficients of oxygen, nitrogen, carbon dioxide, and water vapor in several common polymers.⁵

For some applications, low permeability rates through polymeric materials are desirable, as with food and beverage packaging and automobile tires and inner tubes. Polymer membranes are often used as filters, to selectively separate one chemical species from another (or others) (i.e., the desalination of water). In such instances it is normally the case that the permeation rate of the substance to be filtered is significantly greater than for the other substance(s).

$$P_M = 0.23 \times 10^{-13} \text{ cm}^3 \text{ STP} \cdot \text{cm} / \text{cm}^2 \cdot \text{s} \cdot \text{Pa}$$

$$J = -P_M \frac{\Delta P}{\Delta x}$$

$$= -0.23 \times 10^{-13} \cdot \frac{\text{cm}^3 \text{ STP} \cdot \text{cm}}{\text{cm}^2 \cdot \text{s} \cdot \text{Pa}} \cdot \frac{(0.4 \times 10^5 - 400 \times 10^3) \text{ Pa}}{0.05 \text{ cm}}$$

$$= 1.8 \times 10^{-9} \text{ cm}^3 \text{ STP} / \text{cm}^2 \cdot \text{s}$$

(b)

$$\dot{V}_{CO_2} = JA$$

$$A = 500 \text{ cm}^2, J = 1.8 \times 10^{-9} \text{ cm}^3 \text{ STP} / \text{cm}^2 \cdot \text{s}$$

$$\therefore \dot{V}_{CO_2} = 1.0 \times 10^{-5} \text{ cm}^3 \text{ STP} / \text{s}$$

$$\text{time} = \frac{V}{\dot{V}_{CO_2}} = \frac{750 \text{ cm}^3 \text{ STP}}{1.0 \times 10^{-5} \text{ cm}^3 \text{ STP} / \text{s}} = 8.3 \times 10^6 \text{ s} \approx 97 \text{ days}$$