Materials Science and Engineering I

Chapter 5
Outline of Chapter 5

◆ Rate processes in Solids
◆ Atomic diffusion in solids
◆ Diffusion mechanisms
  - Vacancy or Substitutional Diffusion Mechanism
  - Interstitial Diffusion Mechanism
Steady-state Diffusion
  - Fick’s first law of diffusion
Non-Steady-state Diffusion
  - Fick’s second law of diffusion
Factors affect diffusion
◆ Industrial application of diffusion processes
  - Case hardening of steel by gas carburizing
  - Impurity diffusion into silicon wafers for integrated circuits
◆ Effect of temperature on diffusion in solids
Point Defects

- **Vacancies:**
  - vacant atomic sites in a structure.

- **Self-Interstitials:**
  - "extra" atoms positioned between atomic sites.
Rate Process in Solids

- Reactions occur in solid state resulting in more stable atomic arrangement.
- Reacting atoms must have sufficient energy to overcome activation energy barrier.
- At a given temperature, not all atoms have activation energy $E^*$. It should be supplied to them.

![Diagram showing reaction coordinate with reactants, products, activation energy, and energy released due to reaction.](image)

- $E_r = $ Energy of reactants
- $E^* = $ Activation Energy Level
- $\Delta E^* = $ Activation Energy
- $E_p = $ Energy of Products

Figure 4.33
Rate Process in Solids (Cont..)

- Type equation here. As **temperature** increases, more and more atoms acquire activation energy level.

- **Probability** of finding an atom/molecule with energy \( E^* \) greater than average energy \( E \) of all atoms/ molecules is given by:

\[
e^{-\frac{(E^* - E)}{KT}}
\]

\[K = \text{Boltzman’s Constant} = 1.38 \times 10^{-23} \text{ J/(atom.K)}.
\]

\[T = \text{Temperature in Kelvin}.
\]
The fraction of atoms having energies greater than $E^*$ in a system (when $E^*$ is greater than average energy $E$) is given by

$$\frac{n}{N_{total}} = Ce^{-K.T}$$

$n = \text{Number of molecules greater than energy } E^*$

$N_{total} = \text{Total number of molecules}$

$K = \text{Boltzmann’s Constant}$

$C = \text{Constant}$

$T = \text{Temperature in Kelvin.}$
The number of vacancies at equilibrium at a particular temperature in a metallic crystal lattice is given by

\[ \frac{n_v}{N} = Ce^{\frac{-E_v}{KT}} \]

- \( n_v \) = Number of vacancies per m\(^3\) of metal
- \( E_v \) = Activation Energy to form a vacancy
- \( T \) = Absolute Temperature.
- \( K \) = Boltzmann's Constant.
- \( C \) = Constant
Arrhenius Equation

◆ The rate of chemical reaction is given by Arrhenius equation.

Rate of reaction = \( Ce^{-\frac{Q}{RT}} \)

Q = Activation energy J/mol
R = Molar gas constant J/mol.K
T = Temperature in Kelvin
C = Rate constant (Independent of temperature)

◆ Rate of reaction depends upon number of reacting molecules.
Calculate (a) the equilibrium number of vacancies per cubic meter in pure copper at 500°C and (b) the vacancy fraction at 500°C in pure copper. Assume the energy of formation of a vacancy in pure copper is 0.90 eV. Use Eq. 5.3 with \( C = 1 \). (Boltzmann’s constant \( k = 8.62 \times 10^{-5} \text{ eV/K} \))

**Solution**

a. The equilibrium number of vacancies per cubic meter in pure copper at 500°C is

\[
n_v = Ne^{-E_v/kT} \quad \text{(assume } C = 1 \text{)}
\]

where \( n_v \) = no. of vacancies/m\(^3\)
\( N \) = no. of atom sites/m\(^3\)
\( E_v \) = energy of formation of a vacancy in pure copper at 500°C (eV)
\( k \) = Boltzmann’s constant
\( T \) = temperature (K)

First, we determine a value for \( N \) by using the equation

\[
N = \frac{N_0 \rho_{Cu}}{\text{at. mass Cu}}
\]

where \( N_0 = \text{Avogadro’s number} \) and \( \rho_{Cu} = \text{density of Cu} = 8.96 \text{ Mg/m}^3 \). Thus,

\[
N = \frac{6.02 \times 10^{23} \text{ atoms}}{\text{at. mass}} \times \frac{1}{63.54 \text{ g/at. mass}} \times \frac{8.96 \times 10^5 \text{ g}}{\text{m}^3} = 8.49 \times 10^{28} \text{ atoms/m}^3
\]

Substituting the values of \( N \), \( E_v \), \( k \), and \( T \) into Eq. 5.3a gives

\[
n_v = Ne^{-E_v/kT}
\]

\[
= (8.49 \times 10^{28}) \left\{ \exp \left[-\frac{0.90 \text{ eV}}{(8.62 \times 10^{-5} \text{ eV/K})(773 \text{ K})} \right] \right\}
\]

\[
= (8.49 \times 10^{28})(e^{-13.5}) = (8.49 \times 10^{28})(1.37 \times 10^{-6})
\]

\[= 1.2 \times 10^{23} \text{ vacancies/m}^3\]

b. The vacancy fraction in pure copper at 500°C is found from the ratio \( n_v/N \) from Eq. 5.3a:

\[
n_v/N = \exp \left[-\frac{0.90 \text{ eV}}{(8.62 \times 10^{-5} \text{ eV/K})(773 \text{ K})} \right]
\]

\[= e^{-13.5} = 1.4 \times 10^{-6} \]

Thus, there is only one vacancy in every 10\(^6\) atom sites!
Solidification of Metals

- Arrhenius equation can also be written as
  \[
  \ln \text{(rate)} = \ln (C) - \frac{Q}{RT}
  \]
  Or
  \[
  \log_{10} \text{(rate)} = \log_{10} (C) - \frac{Q}{2.303 RT}
  \]
Which is similar to
\[
Y = b + m X
\]
Which is equation of a **straight line**
With Y intercept as ‘b’ and slope ‘m’.

What is diffusion?

Diffusion is material transport by atomic motion

Inhomogeneous materials can become homogeneous by diffusion. For an active diffusion to occur, the temperature should be high enough to overcome energy barriers to atomic motion.
Atomic Diffusion in Solids

Diffusion is a process by which a matter is transported through another matter.

Examples:

- Movement of smoke particles in air: Very fast.
- Movement of dye in water: Relatively slow.
- Solid state reactions: Very restricted movement due to bonding.
Vacancy diffusion

To jump from lattice site to lattice site, atoms need energy to break bonds with neighbors, and to cause the necessary lattice distortions during jump. This energy comes from the thermal energy of atomic vibrations ($E_{av} \sim kT$)

Materials flow (the atom) is opposite the vacancy flow direction. Diffusion Mechanisms (I) Atom migration Vacancy migration
Vacancy or Substitutional Diffusion mechanism

◆ Atoms diffuse in solids if
  - Vacancies or other crystal defects are present
  - There is enough activation energy

◆ Atoms move into the vacancies present.
◆ More vacancies are created at higher temperature.
◆ Diffusion rate is higher at high temperatures.
Substitutional Diffusion

Example: If atom ‘A’ has sufficient activation energy, it moves into the vacancy → self diffusion.

\[
\text{Activation Energy of Self diffusion} = \text{Activation Energy to form a Vacancy} + \text{Activation Energy to move a vacancy}
\]

As the melting point increases, activation energy also increases.
Interstitial Diffusion mechanism

- Atoms move from one interstitial site to another.
- The atoms that move must be much \textit{smaller} than the matrix atom.
- Example:
  Carbon interstitially diffuses into BCC $\alpha$ or FCC $\gamma$ iron.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure4_37.png}
\caption{Interstitial atom diffusion.}
\label{fig:interstitial_diffusion}
\end{figure}
Steady State Diffusion

- There is no change in concentration of solute atoms at different planes in a system, over a period of time.
- No chemical reaction occurs. Only net flow of atoms.

Net flow of atoms
Per unit area per Unit time = J

Figure 4.38
Fick’s first Law of diffusion

◆ The flux or flow of atoms is given by

\[ J = -D \frac{dc}{dx} \]

- \( J \) = Flux or net flow of atoms.
- \( D \) = Diffusion coefficient.
- \( \frac{dc}{dx} \) = Concentration Gradient.

◆ For steady state diffusion condition, the net flow of atoms by atomic diffusion is equal to diffusion \( D \) times the diffusion gradient \( \frac{dc}{dx} \).

◆ Example: Diffusivity of FCC iron at 500°C is \( 5 \times 10^{-15} \text{ m}^2/\text{S} \) and at 1000°C is \( 3 \times 10^{-11} \text{ m}^2/\text{S} \)

\[
J \left( \frac{\text{atoms}}{\text{m}^2 \cdot \text{s}} \right) = D \left( \frac{\text{m}^2}{\text{s}} \right) \frac{dC}{dx} \left( \frac{\text{atoms}}{\text{m}^3} \times \frac{1}{\text{m}} \right)
\]
Diffusivity depends upon

- **Type of diffusion**: Whether the diffusion is interstitial or substitutional.
- **Temperature**: As the temperature increases, diffusivity increases.
- **Type of crystal structure**: BCC crystal has lower APF than FCC and hence has higher diffusivity.
- **Type of crystal imperfection**: More open structures (grain boundaries) increases diffusion.
- **The concentration of diffusing species**: Higher concentrations of diffusing solute atoms will affect diffusivity.
Non-Steady State Diffusion

- Concentration of solute atoms at any point in metal changes with time in this case.
- Fick’s second law:- Rate of compositional change is equal to diffusivity times the rate of change of concentration gradient.

\[
\frac{dC_x}{dt} = \frac{d}{dx}\left(D \frac{dc_x}{dx}\right)
\]

Change of concentration of solute atoms with change in time in different plane.
Fick’s second law

\[
\frac{J_2 - J_1}{X_2 - X_1} = \frac{C_2 - C_1}{t_2 - t_1}
\]

\[
\Rightarrow \frac{J_2 - J_1}{\Delta X} = \frac{C_2 - C_1}{\Delta t}
\]

\[
\Rightarrow \frac{dJ}{dx} = \frac{dC}{dt}
\]

\[
\Rightarrow d(D\frac{dC}{dx}) = \frac{dC}{dt}
\]

d\[\frac{dC}{dt}\]: Rate of compositional change

d\(D\frac{dC}{dx}\): rate of change of concentration gradient
Fick’s Second Law – Solution

\[
\frac{C_s - C_x}{C_s - C_0} = erf \left( \frac{x}{2\sqrt{D_t}} \right)
\]

- **C_s** = Surface concentration of element in gas diffusing into the surface.
- **C_0** = Initial uniform concentration of element in solid.
- **C_x** = Concentration of element at distance x from surface at time t2.
- **x** = distance from surface
- **D** = diffusivity of solute
- **t** = time.

Table 5.3 Table of the error function

<table>
<thead>
<tr>
<th>z</th>
<th>erf z</th>
<th>z</th>
<th>erf z</th>
<th>z</th>
<th>erf z</th>
<th>z</th>
<th>erf z</th>
<th>z</th>
<th>erf z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0.025</td>
<td>0.0282</td>
<td>0.05</td>
<td>0.0564</td>
<td>0.10</td>
<td>0.1125</td>
<td>0.15</td>
<td>0.1680</td>
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<tr>
<td>0.20</td>
<td>0.2227</td>
<td>0.25</td>
<td>0.2763</td>
<td>0.30</td>
<td>0.3286</td>
<td>0.35</td>
<td>0.3794</td>
<td>0.40</td>
<td>0.4284</td>
</tr>
<tr>
<td>0.45</td>
<td>0.4755</td>
<td>0.50</td>
<td>0.5205</td>
<td>0.55</td>
<td>0.5633</td>
<td>0.6039</td>
<td>0.6039</td>
<td>0.6420</td>
<td>0.6778</td>
</tr>
<tr>
<td>0.70</td>
<td>0.7112</td>
<td>0.75</td>
<td>0.7421</td>
<td>0.80</td>
<td>0.7707</td>
<td>0.8427</td>
<td>0.9340</td>
<td>0.9070</td>
<td>0.9838</td>
</tr>
<tr>
<td>0.85</td>
<td>0.90</td>
<td>0.95</td>
<td>0.9870</td>
<td>1.0</td>
<td>0.9820</td>
<td>1.1</td>
<td>0.8802</td>
<td>1.2</td>
<td>0.9103</td>
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<tr>
<td>1.3</td>
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<td>1.4</td>
<td>0.9523</td>
<td>1.5</td>
<td>0.9661</td>
<td>1.6</td>
<td>0.9763</td>
<td>1.7</td>
<td>0.9838</td>
</tr>
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<td>1.8</td>
<td>0.9891</td>
<td>1.9</td>
<td>0.9928</td>
<td>2.0</td>
<td>0.9933</td>
<td>2.2</td>
<td>0.9998</td>
<td>2.4</td>
<td>0.9999</td>
</tr>
<tr>
<td>2.6</td>
<td>0.9998</td>
<td>2.8</td>
<td>0.9999</td>
<td>3.0</td>
<td>0.9999</td>
<td>3.2</td>
<td>0.9999</td>
<td>3.4</td>
<td>0.9999</td>
</tr>
</tbody>
</table>

\[
D \frac{d^2 C}{dx^2} = \frac{dC}{dt}
\]

Solution:

\[
C = A + B \text{erf} \left( \frac{x}{2\sqrt{Dt}} \right)
\]

Boundary conditions:

\(t=0, \ C=C_0\) at \(X=\infty\)

\(t=\infty, \ C = C_s\) at \(X = 0\)

\(C_0=A + B \text{erf}(\infty) = A + B\)

\(C_s=A + B \text{erf}(0) = A So, \ B=C_0-C_s\)

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

\[
\frac{C_s-C_x}{C_s-C_0} = \text{erf} \left( \frac{x}{2\sqrt{Dt}} \right)
\]
Industrial Applications of Diffusion – Case Hardening

- Sliding and rotating parts need to have hard surfaces.

- These parts are usually machined with low carbon steel as they are easy to machine.

- Their surface is then hardened by carburizing.

- Steel parts are placed at elevated temperature (927°C) in an atmosphere of hydrocarbon gas (CH₄).

- Carbon diffuses into iron surface and fills interstitial space to make it harder.
EXAMPLE PROBLEM 5.2

Consider the gas carburizing of a gear of 1020 steel at 927°C. Calculate the time in minutes necessary to increase the carbon content to 0.40% at 0.50 mm below the surface. Assume that the carbon content at the surface is 0.90% and that the steel has a nominal carbon content of 0.20%.

\[ D_{927°C} = 1.28 \times 10^{-11} \text{ m}^2/\text{s} \]

**Solution**

\[
\frac{C_s - C_x}{C_s - C_0} = \text{erf} \left( \frac{x}{2\sqrt{D_t}} \right)
\]

\[(5.12)\]

\[ C_s = 0.90\% \quad x = 0.5 \text{ mm} = 5.0 \times 10^{-4} \text{ m} \]
\[ C_0 = 0.20\% \quad D_{927°C} = 1.28 \times 10^{-11} \text{ m}^2/\text{s} \]
\[ C_x = 0.40\% \quad t = ? \text{ s} \]

Substituting these values in Eq. 5.12 gives

\[
\frac{0.90 - 0.40}{0.90 - 0.20} = \text{erf} \left( \frac{5.0 \times 10^{-4} \text{ m}}{2\sqrt{(1.28 \times 10^{-11} \text{ m}^2/\text{s})t}} \right)
\]

\[ \frac{0.50}{0.70} = \text{erf} \left( \frac{69.88}{\sqrt{t}} \right) = 0.7143 \]

Let

\[ Z = \frac{69.88}{\sqrt{t}} \quad \text{then erf } Z = 0.7143 \]

We need a number for \( Z \) whose error function (erf) is 0.7143. From Table 5.3 we find this number by interpolation to be 0.755:

\[
\frac{0.7143 - 0.7112}{0.7421 - 0.7112} = \frac{x - 0.75}{0.80 - 0.75}
\]

\[ x - 0.75 = (0.1003)(0.05) \]

\[ x = 0.75 + 0.005 = 0.755 \]

Thus,

\[ Z = \frac{69.88}{\sqrt{t}} = 0.755 \]
\[ \sqrt{t} = \frac{69.88}{0.755} = 92.6 \]
\[ t = 8567 \text{ s} = 143 \text{ min} \]
Consider the gas carburizing of a gear of 1020 steel at 927°C as in Example Problem 5.2. Only in this problem calculate the carbon content at 0.50 mm beneath the surface of the gear after 5 h carburizing time. Assume that the carbon content of the surface of the gear is 0.90% and that the steel has a nominal carbon content of 0.20%.

**Solution**

\[ D_{927°C} = 1.28 \times 10^{-11} \text{ m}^2/\text{s} \]

\[ \frac{C_s - C_x}{C_s - C_0} = \text{erf} \left( \frac{x}{2\sqrt{D_t}} \right) \]  \hspace{1cm} (5.12)

- \( C_s = 0.90\% \)
- \( x = 0.5 \text{ mm} = 5.0 \times 10^{-4} \text{ m} \)
- \( C_0 = 0.20\% \)
- \( D_{927°C} = 1.28 \times 10^{-11} \text{ m}^2/\text{s} \)
- \( C_x = ?\% \)
- \( t = 5 \text{ h} = 5 \times 3600 \text{ s/h} = 1.8 \times 10^4 \text{ s} \)

\[ \frac{0.90 - C_x}{0.90 - 0.20} = \text{erf} \left[ \frac{5.0 \times 10^{-4} \text{ m}}{2\sqrt{(1.28 \times 10^{-11} \text{ m}^2/\text{s})(1.8 \times 10^4 \text{ s})}} \right] \]

\[ \frac{0.90 - C_x}{0.70} = \text{erf} 0.521 \]

Let \( Z = 0.521 \). We need to know what is the corresponding error function for the \( Z \) value of 0.521. To determine this number from Table 5.3, we must interpolate the data as shown in the accompanying table.

<table>
<thead>
<tr>
<th>( Z )</th>
<th>( \text{erf} Z )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.500</td>
<td>0.5205</td>
</tr>
<tr>
<td>0.521</td>
<td>( x )</td>
</tr>
<tr>
<td>0.550</td>
<td>0.5633</td>
</tr>
</tbody>
</table>

\[ \frac{0.521 - 0.500}{0.550 - 0.500} = \frac{x - 0.5205}{0.5633 - 0.5205} \]

\[ 0.42 = \frac{x - 0.5205}{0.0428} \]

\[ x - 0.5205 = (0.42)(0.0428) \]

\[ x = 0.0180 + 0.5205 \]

\[ x = 0.538 \]

Therefore,

\[ \frac{0.90 - C_x}{0.70} = \text{erf} 0.521 = 0.538 \]

\[ C_x = 0.90 - (0.70)(0.538) \]

\[ C_x = 0.52\% \]

Note that by increasing the carburizing time from about 2.4 to 5 h for the 1020 steel, the carbon content at 0.5 mm below the surface of the gear is increased from 0.4% to only 0.52%.
Example Problem 5.4

Consider the impurity diffusion of gallium into a silicon wafer. If gallium is diffused into a silicon wafer with no previous gallium in it at a temperature of 1100°C for 3 h, what is the depth below the surface at which the concentration is $10^{22}$ atoms/m$^3$ if the surface concentration is $10^{24}$ atoms/m$^3$? For gallium diffusing into silicon at 1100°C the solution is as follows:

**Solution**

\[ D_{1100°C} = 7.0 \times 10^{-17} \text{ m}^2/\text{s} \]

\[ \frac{C_s - C_x}{C_s - C_0} = \text{erf} \left( \frac{x}{2 \sqrt{Dt}} \right) \]  \hspace{1cm} \text{(5.12)}

- \( C_s = 10^{24} \text{ atoms/m}^3 \)
- \( x = ? \text{m} \) (depth at which \( C_x = 10^{22} \text{ atoms/m}^3 \))
- \( C_x = 10^{22} \text{ atoms/m}^3 \)
- \( D_{1100°C} = 7.0 \times 10^{-17} \text{ m}^2/\text{s} \)
- \( C_0 = 0 \text{ atoms/m}^3 \)
- \( t = 3 \text{ h} \times 3600 \text{ s/h} = 1.08 \times 10^4 \text{ s} \)

Substituting these values into Eq. 5.12 gives

\[ \frac{10^{24} - 10^{22}}{10^{24} - 0} = \text{erf} \left( \frac{x \text{ m}}{2 \sqrt{(7.0 \times 10^{-17} \text{m}^2/\text{s})(1.08 \times 10^4 \text{ s})}} \right) \]

\[ 1 - 0.01 = \text{erf} \left( \frac{x \text{ m}}{1.74 \times 10^{-6} \text{ m}} \right) = 0.99 \]

Let

\[ Z = \frac{x}{1.74 \times 10^{-6} \text{ m}} \]

Thus,

\[ \text{erf} Z = 0.99 \quad \text{and} \quad Z = 1.82 \]

(from Table 5.3 using interpolation). Therefore,

\[ x = (Z)(1.74 \times 10^{-6} \text{ m}) = (1.82)(1.74 \times 10^{-6} \text{ m}) \]

\[ = 3.17 \times 10^{-6} \text{ m} \]
Carburizing

Low carbon steel part

Diffusing carbon atoms

Carbon Gradients in Carburized metals
Impurity Diffusion into Silicon wafer

- Impurities are made to diffuse into silicon wafer to change its electrical characteristics.
- Used in integrated circuits.
- Silicon wafer is exposed to vapor of impurity at 1100°C in a quartz tube furnace.
- The concentration of impurity at any point depends on depth and time of exposure.

Figure 4.44

Effect of Temperature on Diffusion

**Dependence of rate of diffusion on temperature is given by**

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

or

\[ \ln D = \ln D_0 - \frac{Q}{RT} \]

or

\[ \log_{10} D = \log_{10} D_0 - \frac{Q}{2.303RT} \]

- **D** = Diffusivity m²/S
- **D₀** = Proportionality constant m²/S
- **Q** = Activation energy of diffusing species J/mol
- **R** = Molar gas constant = 8.314 J/mol.K
- **T** = Temperature (K)
Effect of Temperature on Diffusion-Example

◆ If diffusivity at two temperatures are determined, two equations can be solved for $Q$ and $D_0$

◆ Example:-

The diffusivity of silver atoms in silver is $1 \times 10^{-17}$ at $500^0C$ and $7 \times 10^{-13}$ at $1000^0C$.

Therefore,

$$\frac{D_{1000}}{D_{500}} = \frac{\exp(-Q / RT_2)}{\exp(-Q / RT_1)} = \exp\left(-\frac{Q}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)\right)$$

$$\frac{7 \times 10^{-13}}{1 \times 10^{-17}} = \exp\left(-\frac{Q}{R}\left(\frac{1}{1273} - \frac{1}{773}\right)\right)$$

Solving for activation energy $Q$

$$Q = 183 KJ / mol$$
The diffusivity of silver atoms in solid silver metal is $1.0 \times 10^{-17}$ m$^2$/s at 500°C and $7.0 \times 10^{-13}$ m$^2$/s at 1000°C. Calculate the activation energy (joules per mole) for the diffusion of Ag in Ag in the temperature range 500°C to 1000°C.

**Solution**

Using Eq. 5.13, $T_2 = 1000^\circ\text{C} + 273 = 1273 \text{ K}$, $T_1 = 500^\circ\text{C} + 273 = 773 \text{ K}$, and $R = 8.314 \text{ J/(mol \cdot K)}$:

$$\frac{D_{1000^\circ\text{C}}}{D_{500^\circ\text{C}}} = \frac{\exp(-Q/RT_2)}{\exp(-Q/RT_1)} = \exp\left[\frac{Q}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)\right]$$

$$\frac{7.0 \times 10^{-13}}{1.0 \times 10^{-17}} = \exp\left\{\frac{Q}{R}\left[\left(\frac{1}{1273 \text{ K}} - \frac{1}{773 \text{ K}}\right)\right]\right\}$$

$$\ln (7.0 \times 10^4) = \frac{Q}{R} (7.855 \times 10^{-4} - 12.94 \times 10^{-4}) = \frac{Q}{8.314} (5.08 \times 10^{-4})$$

$11.16 = Q (6.11 \times 10^{-5})$

$Q = 183,000 \text{ J/mol} = 183 \text{ kJ/mol}$
Example Problem 5.6

Calculate the value of the diffusivity $D$ in meters squared per second for the diffusion of carbon in $\gamma$ iron (FCC) at 927°C. Use values of $D_0 = 2.0 \times 10^{-5} \text{ m}^2/\text{s}$, $Q = 142 \text{ kJ/mol}$, and $R = 8.314 \text{ J/(mol} \cdot \text{K)}$.

**Solution**

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

\[
= (2.0 \times 10^{-5} \text{ m}^2/\text{s}) \left\{ \exp \left[ \frac{-142,000 \text{ J/mol}}{[8.314 \text{ J/(mol} \cdot \text{K}] (1200 \text{ K})} \right] \right\}
\]

\[
= (2.0 \times 10^{-5} \text{ m}^2/\text{s}) (e^{-14.23})
\]

\[
= (2.0 \times 10^{-5} \text{ m}^2/\text{s}) (0.661 \times 10^{-6})
\]

\[
= 1.32 \times 10^{-11} \text{ m}^2/\text{s}
\]