Problems

Section 5-1 Applications of Diffusion
5-1 What is the driving force for diffusion?
5-2 In the carburization treatment of steels, what are the diffusing species?
5-3 Why do we use PET plastic to make carbonated beverage bottles?
5-4 Why is it that aluminum metal oxidizes more readily than iron but aluminum is considered to be a metal that usually does not “rust?”
5-5 What is a thermal barrier coating? Where are such coatings used?

Section 5-2 Stability of Atoms and Ions
5-6 What is a nitriding heat treatment?
5-7 A certain mechanical component is heat treated using carburization. A common engineering problem encountered is that we need to machine a certain part of the component and this part of the surface should not be hardened. Explain how we can achieve this objective.
5-8 Write down the Arrhenius equation and explain the different terms.
5-9 Atoms are found to move from one lattice position to another at the rate of $5 \times 10^5$ jumps at 400°C when the activation energy for their movement is 30,000 cal/mol. Calculate the jump rate at 750°C.
5-10 The number of vacancies in a material is related to temperature by an Arrhenius equation. If the fraction of lattice points containing vacancies is $8 \times 10^{-5}$ at 600°C, determine the fraction of lattice points containing vacancies at 1000°C.
5-11 The Arrhenius equation was originally developed for comparing rates of chemical reactions. Compare the rates of a chemical reaction at 20 and 100°C by calculating the ratio of the chemical reaction rates. Assume that the activation energy for liquids in which the chemical reaction is conducted is 10 kJ/mol and that the reaction is limited by diffusion.

Section 5-3 Mechanisms for Diffusion
5-12 What are the different mechanisms for diffusion?

Section 5-4 Activation Energy for Diffusion
5-13 Why is it that the activation energy for diffusion via the interstitial mechanism is smaller than those for other mechanisms?
5-14 How is self-diffusion of atoms in metals verified experimentally?
5-15 Compare the diffusion coefficients of carbon in BCC and FCC iron at the allotropic transformation temperature of 912°C and explain the difference.
5-16 Compare the diffusion coefficients for hydrogen and nitrogen in FCC iron at 1000°C and explain the difference.

Section 5-5 Rate of Diffusion
(Fick’s First Law)
5-17 Activation energy is sometimes expressed as (eV/atom). For example, see Figure 5-15 illustrating the diffusion coefficients of ions in different oxides. Convert eV/atom into Joules/mole.
5-18 The diffusion coefficient for Cr$^{3+}$ in Cr$_2$O$_3$ is $6 \times 10^{-15}$ cm$^2$/s at 727°C and $1 \times 10^{-9}$ cm$^2$/s at 1400°C. Calculate
   (a) the activation energy and
   (b) the constant $D_0$.
5-19 The diffusion coefficient for O$^{2-}$ in Cr$_2$O$_3$ is $4 \times 10^{-15}$ cm$^2$/s at 1150°C and $6 \times 10^{-11}$ cm$^2$/s at 1715°C. Calculate
   (a) the activation energy and
   (b) the constant $D_0$.
5-20 Without referring to the actual data, can you predict whether the activation energy for diffusion of carbon in FCC iron will be higher or lower than that in BCC iron? Explain.

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Problems

If the flux of nitrogen through the foil is $10^{12}$ atoms/(cm$^2 \cdot$ s), what is the nitrogen concentration in the low concentration region?

5-24 A 0.2-mm-thick wafer of silicon is treated so that a uniform concentration gradient of antimony is produced. One surface contains 1 Sb atom per $10^8$ Si atoms and the other surface contains 500 Sb atoms per $10^8$ Si atoms. The lattice parameter for Si is 5.4307 Å (Appendix A). Calculate the concentration gradient in
(a) atomic percent Sb per cm and
(b) Sb atoms/cm$^3$.

5-25 When a Cu-Zn alloy solidifies, one portion of the structure contains 25 atomic percent zinc and another portion 0.025 mm away contains 20 atomic percent zinc. The lattice parameter for the FCC alloy is about 3.63 $\times$ 10$^{-8}$ cm. Determine the concentration gradient in
(a) atomic percent Zn per cm;
(b) weight percent Zn per cm; and
(c) Zn atoms/cm$^3$.

5-26 A 0.001 in. BCC iron foil is used to separate a high hydrogen content gas from a low hydrogen content gas at 650°C. $5 \times 10^8$ H atoms/cm$^3$ are in equilibrium on one side of the foil, and $2 \times 10^3$ H atoms/cm$^3$ are in equilibrium with the other side. Determine
(a) the concentration gradient of hydrogen and
(b) the flux of hydrogen through the foil.

5-27 A 1-mm-thick sheet of FCC iron is used to contain nitrogen in a heat exchanger at 1200°C. The concentration of N at one surface is 0.04 atomic percent, and the concentration at the second surface is 0.005 atomic percent. Determine the flux of nitrogen through the foil in N atoms/(cm$^2 \cdot$ s).

5-28 A 4-cm-diameter, 0.5-mm-thick spherical container made of BCC iron holds nitrogen at 700°C. The concentration at the inner surface is 0.05 atomic percent and at the outer surface is 0.002 atomic percent. Calculate the number of grams of nitrogen that are lost from the container per hour.

5-29 A BCC iron structure is to be manufactured that will allow no more than 50 g of hydrogen to be lost per year through each square centimeter of the iron at 400°C. If the concentration of hydrogen at one surface is 0.05 H atom per unit cell and 0.001 H atom per unit cell at the second surface, determine the minimum thickness of the iron.

5-30 Determine the maximum allowable temperature that will produce a flux of less than 2000 H atoms/(cm$^2 \cdot$ s) through a BCC iron foil when the concentration gradient is $-5 \times 10^{16}$ atoms/cm$^3$. (Note the negative sign for the flux.)

Section 5-6 Factors Affecting Diffusion

5-31 Write down the equation that describes the dependence of $D$ on temperature.

5-32 In solids, the process of diffusion of atoms and ions takes time. Explain how this is used to our advantage while forming metallic glasses.

5-33 Why is it that inorganic glasses form upon relatively slow cooling of melts, while rapid solidification is necessary to form metallic glasses?

5-34 Use the diffusion data in the table below for atoms in iron to answer the questions that follow. Assume metastable equilibrium conditions and trace amounts of C in Fe. The gas constant in SI units is 8.314 J/(mol $\cdot$ K).

<table>
<thead>
<tr>
<th>Diffusion Couple</th>
<th>Diffusion Mechanism</th>
<th>$Q$ (J/mol)</th>
<th>$D_0$ (m$^2$/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C in FCC iron</td>
<td>Interstitial</td>
<td>$1.38 \times 10^6$</td>
<td>$2.3 \times 10^{-5}$</td>
</tr>
<tr>
<td>C in BCC iron</td>
<td>Interstitial</td>
<td>$8.74 \times 10^4$</td>
<td>$1.1 \times 10^{-6}$</td>
</tr>
<tr>
<td>Fe in FCC iron</td>
<td>Vacancy</td>
<td>$2.79 \times 10^5$</td>
<td>$6.5 \times 10^{-5}$</td>
</tr>
<tr>
<td>Fe in BCC iron</td>
<td>Vacancy</td>
<td>$2.46 \times 10^5$</td>
<td>$4.1 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

(a) Plot the diffusion coefficient as a function of inverse temperature ($1/T$) showing all four diffusion couples in the table.
(b) Recall the temperatures for phase transitions in iron, and for each case, indicate on the graph the temperature range over which the diffusion data is valid.
(c) Why is the activation energy for Fe diffusion higher than that for C diffusion in iron?
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5-35 The plot above has three lines representing grain boundary, surface, and volume self-diffusion in a metal. Match the lines labeled A, B, and C with the type of diffusion. Justify your answer by calculating the activation energy for diffusion for each case.

Section 5-7 Permeability of Polymers

5-36 What are barrier polymers?

5-37 What factors, other than permeability, are important in selecting a polymer for making plastic bottles?

5-38 Amorphous PET is more permeable to CO$_2$ than PET that contains microcrystallites. Explain why.

Section 5-8 Composition Profile (Fick’s Second Law)

5-39 Transistors are made by doping single crystal silicon with different types of impurities to generate n- and p-type regions. Phosphorus (P) and boron (B) are typical n- and p-type dopant species, respectively. Assuming that a thermal treatment at 1100°C for 1 h is used to cause diffusion of the dopants, calculate the constant surface concentration of P and B needed to achieve a concentration of $10^{18}$ atoms/cm$^3$ at a depth of 0.1 μm from the surface for both n- and p-type regions. The diffusion coefficients of P and B in single crystal silicon at 1100°C are $6.5 \times 10^{-13}$ cm$^2$/s and $6.1 \times 10^{-13}$ cm$^2$/s, respectively.

5-40 Consider a 2-mm-thick silicon (Si) wafer to be doped using antimony (Sb). Assume that the dopant source (gas mixture of antimony chloride and other gases) provides a constant concentration of $10^{22}$ atoms/m$^3$. We need a dopant profile such that the concentration of Sb at a depth of 1 micrometer is $5 \times 10^{21}$ atoms/m$^3$. What is the required time for the diffusion heat treatment? Assume that the silicon wafer initially contains no impurities or dopants. Assume that the activation energy for diffusion of Sb in silicon is 380 kJ/mole and $D_0$ for Sb diffusion in Si is $1.3 \times 10^{-13}$ cm$^2$/s. Assume $T = 1250°C$.

5-41 Consider doping of Si with gallium (Ga). Assume that the diffusion coefficient of gallium in Si at 1100°C is $7 \times 10^{-13}$ cm$^2$/s. Calculate the concentration of Ga at a depth of 2.0 micrometer if the surface concentration of Ga is $10^{23}$ atoms/cm$^3$. The diffusion times are 1, 2, and 3 hours.

5-42 Compare the rate at which oxygen ions diffuse in alumina (Al$_2$O$_3$) with the rate at which aluminum ions diffuse in Al$_2$O$_3$ at 1500°C. Explain the difference.

5-43 A carburizing process is carried out on a 0.10% C steel by introducing 1.0% C at the surface at 980°C, where the iron is FCC. Calculate the carbon content at 0.01 cm, 0.05 cm, and 0.10 cm beneath the surface after 1 h.

5-44 Iron containing 0.05% C is heated to 912°C in an atmosphere that produces 1.20% C at the surface and is held for 24 h. Calculate the carbon content at 0.05 cm beneath the surface if (a) the iron is BCC and (b) the iron is FCC. Explain the difference.

5-45 What temperature is required to obtain 0.50% C at a distance of 0.5 mm beneath the surface of a 0.20% C steel in 2 h, when 1.10% C is present at the surface? Assume that the iron is FCC.

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5-46 A 0.15% C steel is to be carburized at 1100°C, giving 0.35% C at a distance of 1 mm beneath the surface. If the surface composition is maintained at 0.90% C, what time is required?

5-47 A 0.02% C steel is to be carburized at 1200°C in 4 h, with the carbon content 0.6 mm beneath the surface reaching 0.45% C. Calculate the carbon content required at the surface of the steel.

5-48 A 1.2% C tool steel held at 1150°C is exposed to oxygen for 48 h. The carbon content at the steel surface is zero. To what depth will the steel be decarburized to less than 0.20% C?

5-49 A 0.80% C steel must operate at 950°C in an oxidizing environment for which the carbon content at the steel surface is zero. Only the outermost 0.02 cm of the steel part can fall below 0.75% C. What is the maximum time that the steel part can operate?

5-50 A steel with the BCC crystal structure containing 0.001% N is nitrided at 550°C for 5 h. If the nitrogen content at the steel surface is 0.08%, determine the nitrogen content at 0.25 mm from the surface.

5-51 What time is required to nitride a 0.002% N steel to obtain 0.12% N at a distance of 0.002 in. beneath the surface at 625°C? The nitrogen content at the surface is 0.15%.

5-52 We can successfully perform a carburizing heat treatment at 1200°C in 1 h. In an effort to reduce the cost of the brick lining in our furnace, we propose to reduce the carburizing temperature to 950°C. What time will be required to give us a similar carburizing treatment?

5-53 During freezing of a Cu-Zn alloy, we find that the composition is nonuniform. By heating the alloy to 600°C for 3 h, diffusion of zinc helps to make the composition more uniform. What temperature would be required if we wished to perform this homogenization treatment in 30 minutes?

5-54 To control junction depth in transistors, precise quantities of impurities are introduced at relatively shallow depths by ion implantation and diffused into the silicon substrate in a subsequent thermal treatment. This can be approximated as a finite source diffusion problem. Applying the appropriate boundary conditions, the solution to Fick’s second law under these conditions is

\[ c(x, t) = \frac{Q}{\sqrt{\pi Dt}} \exp\left(\frac{x^2}{4Dt}\right), \]

where \( Q \) is the initial surface concentration with units of atoms/cm². Assume that we implant \( 10^{14} \text{ atoms/cm}^2 \) of phosphorus at the surface of a silicon wafer with a background boron concentration of \( 10^{16} \text{ atoms/cm}^3 \) and this wafer is subsequently annealed at 1100°C. The diffusion coefficient \( (D) \) of phosphorus in silicon at 1100°C is \( 6.5 \times 10^{-13} \text{ cm}^2/\text{s} \).

(a) Plot a graph of the concentration \( c \) (atoms/cm³) versus \( x \) (cm) for anneal times of 5 minutes, 10 minutes, and 15 minutes.

(b) What is the anneal time required for the phosphorus concentration to equal the boron concentration at a depth of 1 μm?

Section 5-9 Diffusion and Materials Processing

5-55 Arrange the following materials in increasing order of self-diffusion coefficient: Ar gas, water, single crystal aluminum, and liquid aluminum at 700°C.

5-56 Most metals and alloys can be processed using the melting and casting route, but we typically do not choose to apply this method for the processing of specific metals (e.g., W) and most ceramics. Explain.

5-57 What is sintering? What is the driving force for sintering?

5-58 Why does grain growth occur? What is meant by the terms normal and abnormal grain growth?

5-59 Why is the strength of many metallic materials expected to decrease with increasing grain size?

5-60 A ceramic part made of MgO is sintered successfully at 1700°C in 90 minutes. To minimize thermal stresses during the process, we plan to reduce the temperature to 1500°C. Which will limit the rate at which sintering can be done: diffusion of magnesium ions or...