



Properties of Engineering Materials Diffusion

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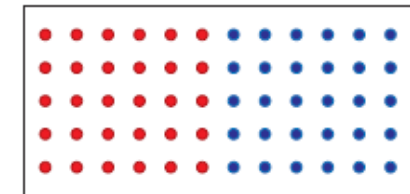
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Introduction

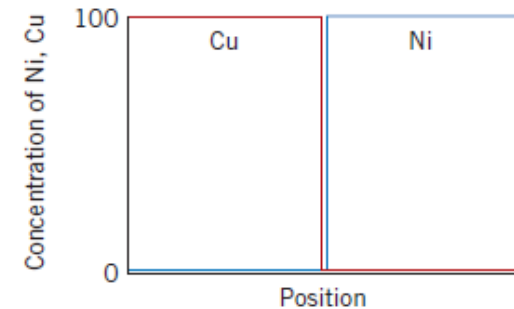
- **Diffusion:** the phenomenon of material transport by atomic motion; it is the transfer of mass either within a specific solid or from a liquid, a gas, or another solid phase.
 - Let's consider the diffusion couple shown in Fig. 5.1. This represents the metals before heating.



(a)



(b)



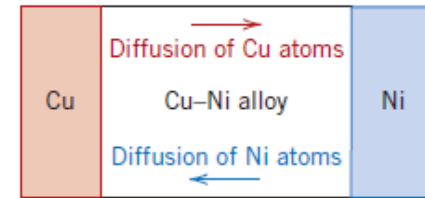
(c)

Figure 5.1 (a) A copper–nickel diffusion couple before a high-temperature heat treatment. (b) Schematic representations of Cu (red circles) and Ni (blue circles) atom locations within the diffusion couple. (c) Concentrations of copper and nickel as a function of position across the couple.

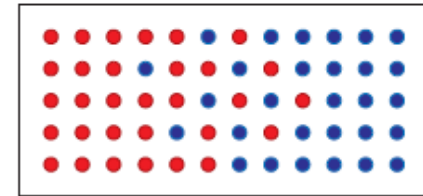
Introduction

- **Diffusion**: the phenomenon of material transport by atomic motion; it is the transfer of mass either within a specific solid or from a liquid, a gas, or another solid phase.
 - Now consider the same couple shown in Fig. 5.2 after heating to a temperature below the melting point of the two metals for an extended period of time.

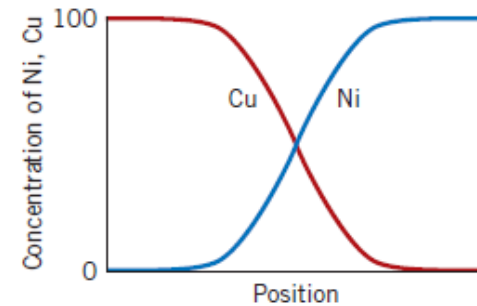
Cu atoms have migrated or diffused into the Ni, and that Ni has diffused into Cu (**Interdiffusion**).



(a)



(b)



(c)

Figure 5.2 (a) A copper–nickel diffusion couple after a high-temperature heat treatment, showing the alloyed diffusion zone. (b) Schematic representations of Cu (red circles) and Ni (blue circles) atom locations within the couple. (c) Concentrations of copper and nickel as a function of position across the couple.



Diffusion Mechanisms

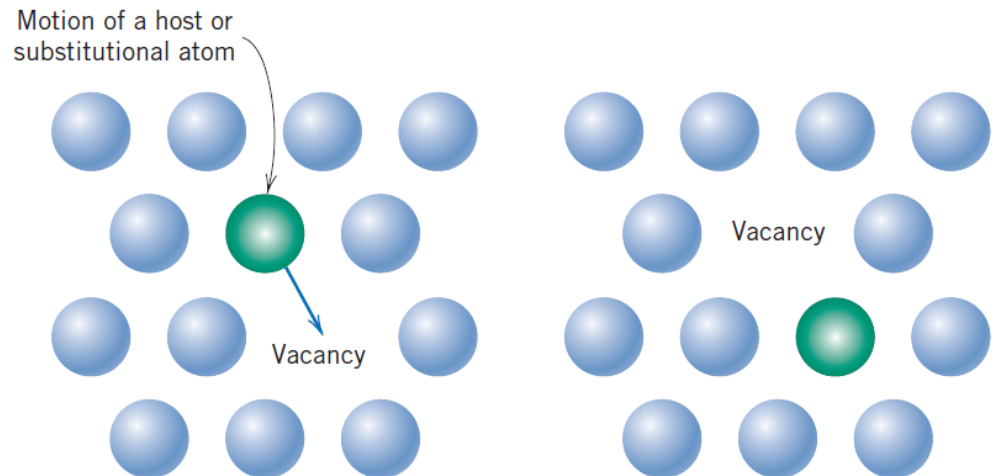
- From an atomic perspective, diffusion is just the stepwise migration of atoms from lattice site to lattice site.
- In fact, the atoms in solid materials are in constant motion, rapidly changing positions.
- For an atom to make such a move, two conditions must be met:
 - (1) there must be an empty adjacent site, and
 - (2) the atom must have sufficient energy to break bonds with its neighbor atoms and then cause some lattice distortion during the displacement.

Diffusion Mechanisms

- Two models for atomic motion:
 - **Vacancy Diffusion:** the interchange of an atom from a normal lattice position to an adjacent vacant lattice site or vacancy.
 - The higher the temperature the more the vacant sites and the higher the ability of an atom to diffuse (as it possesses higher energy).

The vacancy moves in a direction opposite to that of the atom's.

Both self-diffusion (within one metal) and interdiffusion occur by this mechanism.



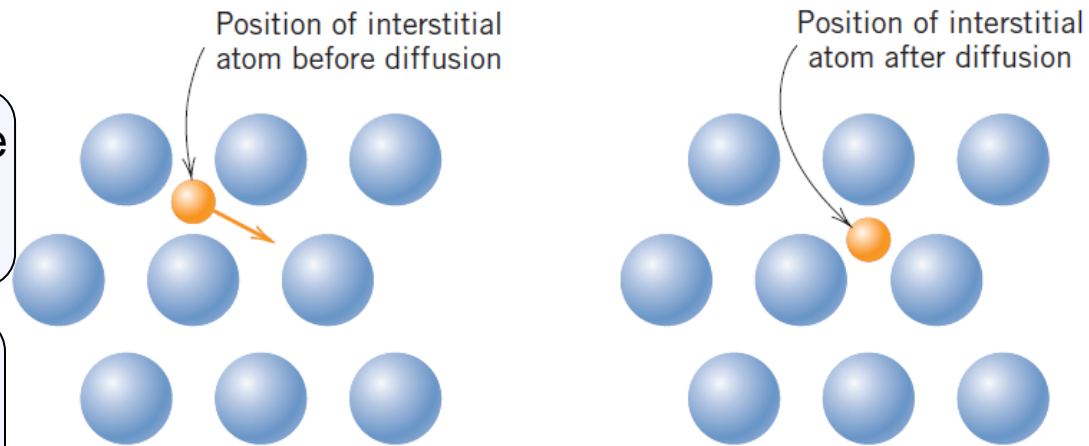
(a)

Diffusion Mechanisms

- Two models for atomic motion:
 - **Interstitial Diffusion:** interdiffusion of impurities such as H, C, N, and O, which have atoms that are small enough to fit into the interstitial positions.
 - Involves atoms that migrate from an interstitial position to a neighboring one that is empty.

Interstitial diffusion occurs much more rapidly than diffusion by the vacancy mode.

Interstitial atoms are small and more mobile, and there are more empty interstitial positions than vacancies.



(b)

Processing Using Diffusion

- **Case Hardening:**
 - Diffuse carbon atoms into the host iron atoms at the surface.
 - Example of interstitial diffusion is a case hardened gear.

- **Result:** The presence of C atoms makes iron (steel) harder.



Adapted from chapter-opening photograph, Chapter 5, *Callister & Rethwisch 8e*. (Courtesy of Surface Division, Midland-Ross.)

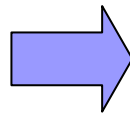
Steady – State Diffusion

- **Diffusion flux** (J in $\text{kg}/\text{m}^2\cdot\text{s}$ or $\text{atoms}/\text{m}^2\cdot\text{s}$): a term used to describe how fast diffusion occurs. It is defined as the mass M diffusing through and perpendicular to a unit cross-sectional area of solid per unit of time.

$$J = \frac{M}{At}$$

A denotes the area across which diffusion is occurring and t is the elapsed diffusion time.

$$J = \frac{1}{A} \frac{dM}{dt}$$

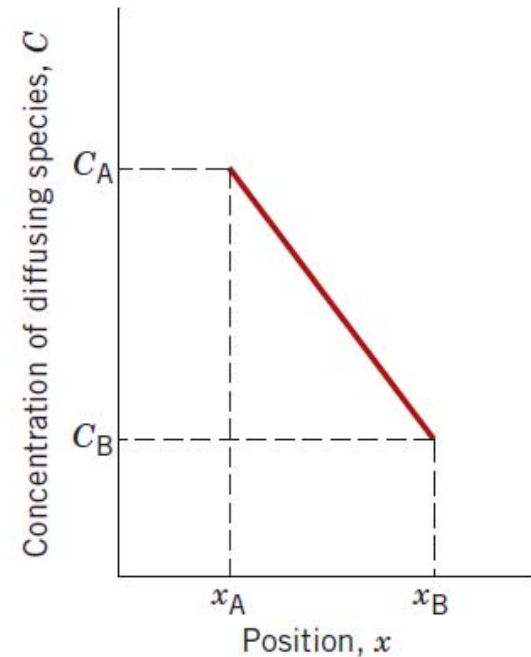
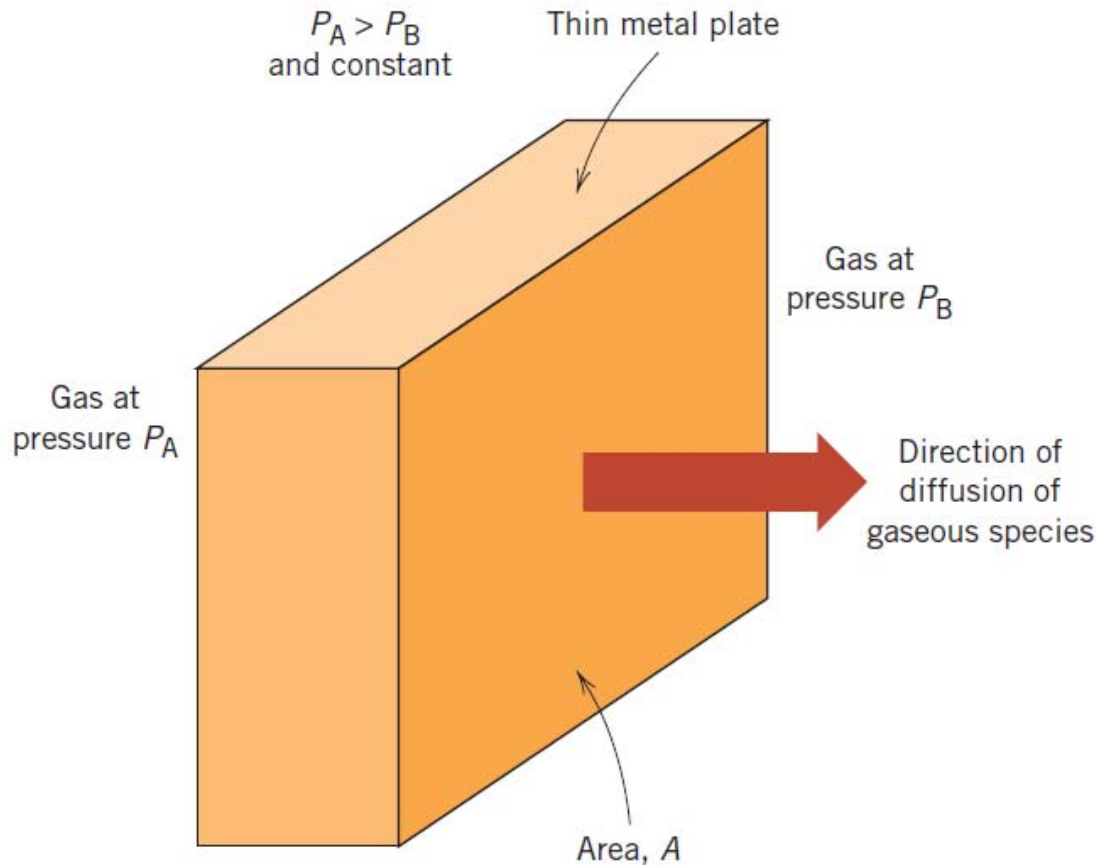


In differential form

Steady – State Diffusion

- **Steady-state diffusion:** one in which diffusion flux does not change with time.
 - Example is the diffusion of atoms of a gas through a plate of metal for which the concentrations (or pressures) of the diffusing species on both surfaces of the plate are held constant.

Steady – State Diffusion



(a)

(b)

Figure 5.4 (a) Steady-state diffusion across a thin plate. (b) A linear **concentration profile** for the diffusion situation in (a).

Steady – State Diffusion

Concentration gradient: the slope at a particular point on this curve.

$$\text{concentration gradient} = \frac{dC}{dx}$$

If concentration profile is linear



$$\text{concentration gradient} = \frac{\Delta C}{\Delta x} = \frac{C_A - C_B}{x_A - x_B}$$

The flux is proportional to the concentration gradient

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

D : diffusion coefficient (m²/s).

Fick's first law

Steady – State Diffusion

- One practical example of steady-state diffusion is found in the purification of hydrogen gas.
 - One side of a thin sheet of palladium metal is exposed to the impure gas composed of hydrogen and other gaseous species such as nitrogen, oxygen, and water vapor.
 - The hydrogen selectively diffuses through the sheet to the opposite side, which is maintained at a constant and lower hydrogen pressure.



Steady – State Diffusion

- Example 5.1: Diffusion Flux Computation

Nonsteady – State Diffusion

- Most practical diffusion situations are nonsteady-state ones.
 - That is, the diffusion flux and the concentration gradient at some particular point in a solid vary with time

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial C}{\partial x} \right) \quad \text{Fick's second law}$$

If D is independent of composition $\longrightarrow \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$

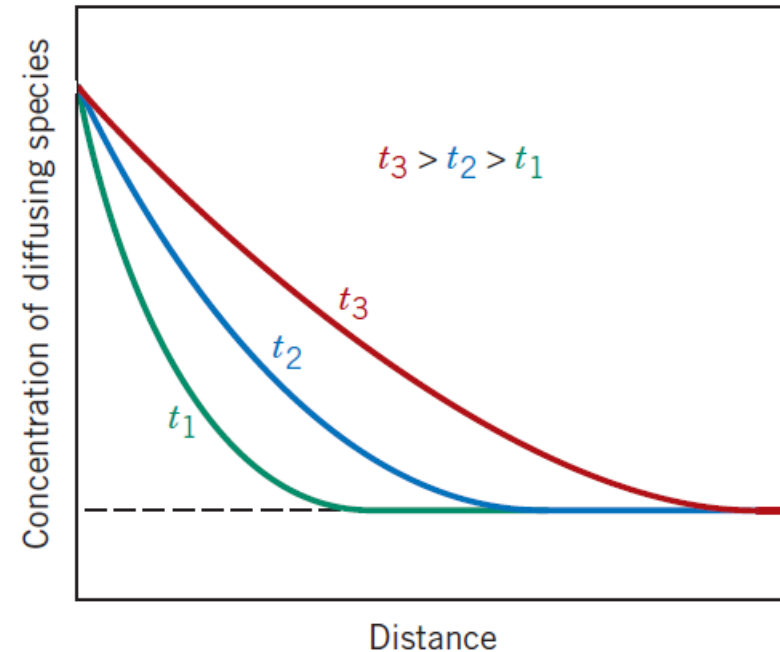
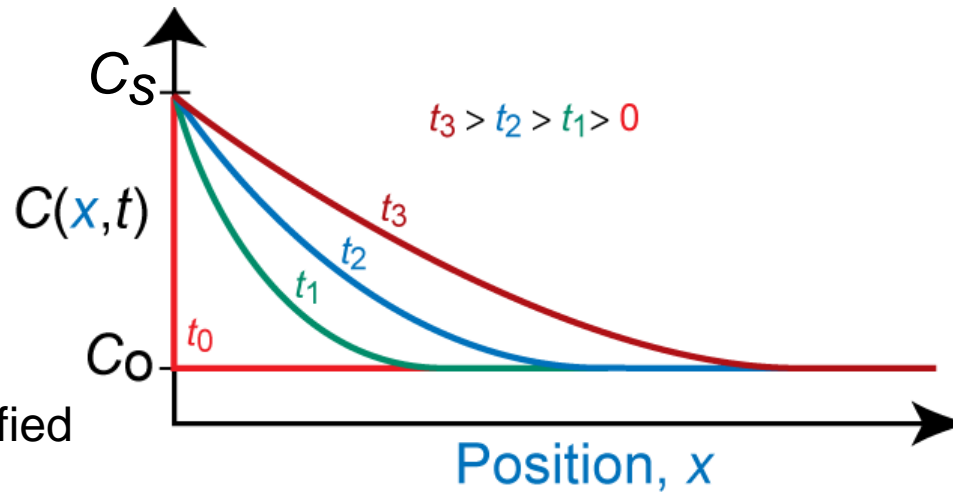
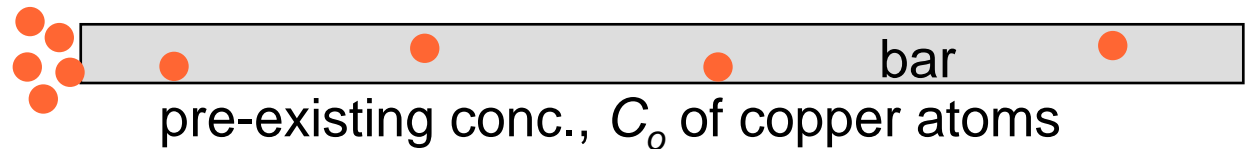


Figure 5.5 Concentration profiles for nonsteady-state diffusion taken at three different times.

Nonsteady – State Diffusion

- Copper diffuses into a bar of aluminum.

Surface conc.,
 C_S of Cu atoms



B.C. at $t = 0$, $C = C_o$ for $0 \leq x \leq \infty$

at $t > 0$, $C = C_S$ for $x = 0$ (constant surface conc.)

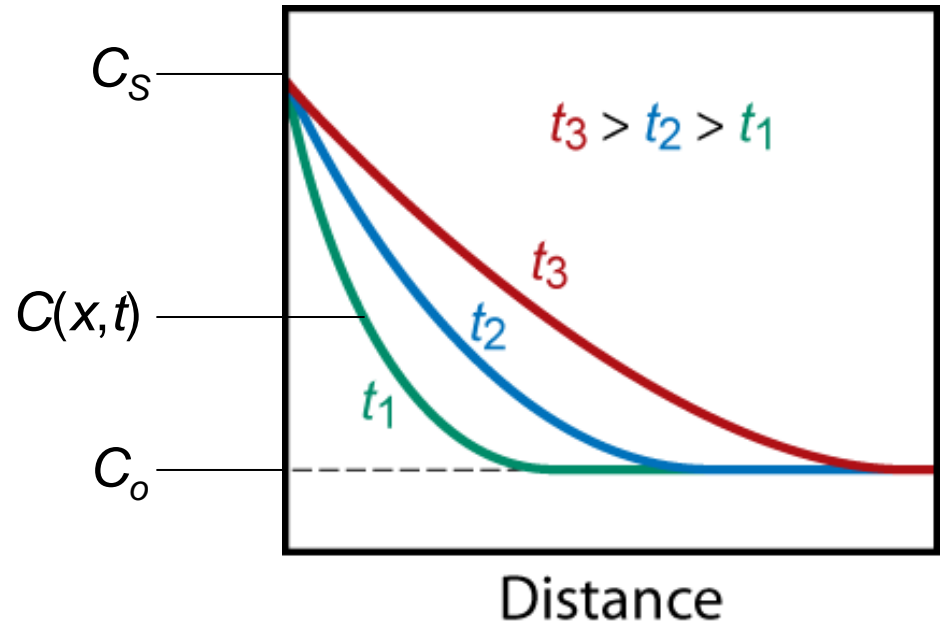
$C = C_o$ for $x = \infty$

Nonsteady – State Diffusion

- Applying B.C. to Fick's second law yields the following:

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

Error function





Nonsteady – State Diffusion

- Example 5.2:



Nonsteady – State Diffusion

- Example 5.3:

Factors That Influence Diffusion

Diffusing Species

- The higher the diffusion coefficient (D) the higher the rate at which the atoms diffuse.
- The diffusing species as well as the host material influence the diffusion coefficient.
 - For example, there is a significant difference in magnitude between self-diffusion and carbon interdiffusion in α iron at 500°C , the D value being greater for the carbon interdiffusion.
- Self-diffusion occurs by a vacancy mechanism, whereas carbon diffusion in iron is interstitial.

Factors That Influence Diffusion

Diffusing Species

<i>Diffusing Species</i>	<i>Host Metal</i>	<i>D₀(m²/s)</i>	<i>Activation Energy Q_a</i>		<i>Calculated Value</i>	
			<i>kJ/mol</i>	<i>eV/atom</i>	<i>T(°C)</i>	<i>D(m²/s)</i>
Fe	α-Fe (BCC)	2.8×10^{-4}	251	2.60	500	3.0×10^{-21}
					900	1.8×10^{-15}
Fe	γ-Fe (FCC)	5.0×10^{-5}	284	2.94	900	1.1×10^{-17}
					1100	7.8×10^{-16}
C	α-Fe	6.2×10^{-7}	80	0.83	500	2.4×10^{-12}
					900	1.7×10^{-10}
C	γ-Fe	2.3×10^{-5}	148	1.53	900	5.9×10^{-12}
					1100	5.3×10^{-11}
Cu	Cu	7.8×10^{-5}	211	2.19	500	4.2×10^{-19}
Zn	Cu	2.4×10^{-5}	189	1.96	500	4.0×10^{-18}
Al	Al	2.3×10^{-4}	144	1.49	500	4.2×10^{-14}
Cu	Al	6.5×10^{-5}	136	1.41	500	4.1×10^{-14}
Mg	Al	1.2×10^{-4}	131	1.35	500	1.9×10^{-13}
Cu	Ni	2.7×10^{-5}	256	2.65	500	1.3×10^{-22}

Table 5.2 A Tabulation of Diffusion Data

Factors That Influence Diffusion

Temperature

- Temperature has a most profound influence on the coefficients and diffusion rates.
 - For example, for the self-diffusion of Fe in α -Fe, the diffusion coefficient increases approximately six orders of magnitude on rising temperature from 500° C to 900° C.
- The temperature dependence of the diffusion coefficient is:

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

D_0 = a temperature-independent preexponential (m²/s)
 Q_d = the **activation energy** for diffusion (J/mol or eV/atom)
 R = the gas constant, 8.31 J/mol.K or 8.62×10^{-5} eV/atom.K
 T = absolute temperature (K)



Factors That Influence Diffusion

Temperature

- Example 5.4: