Chapter Outline

Diffusion - how do atoms move through solids?

- **Diffusion mechanisms**
  - **Vacancy diffusion**
  - **Interstitial diffusion**
  - **Impurities**

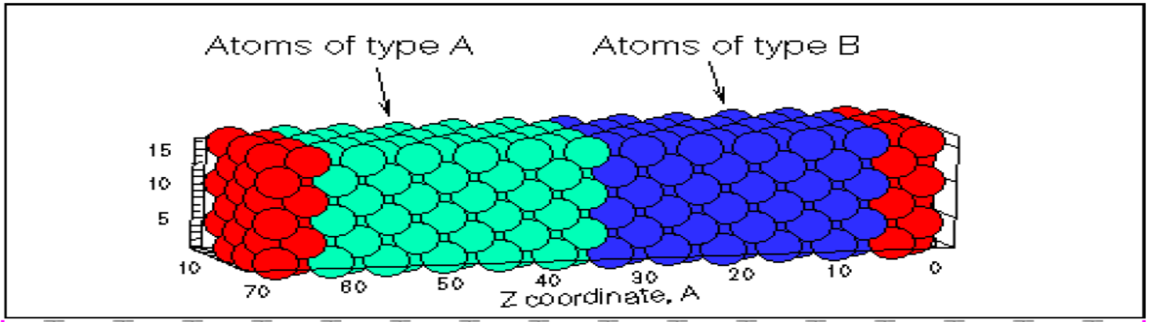
- **The mathematics of diffusion**
  - **Steady-state diffusion (Fick's first law)**
  - *Nonsteady-State Diffusion (Fick's second law)*

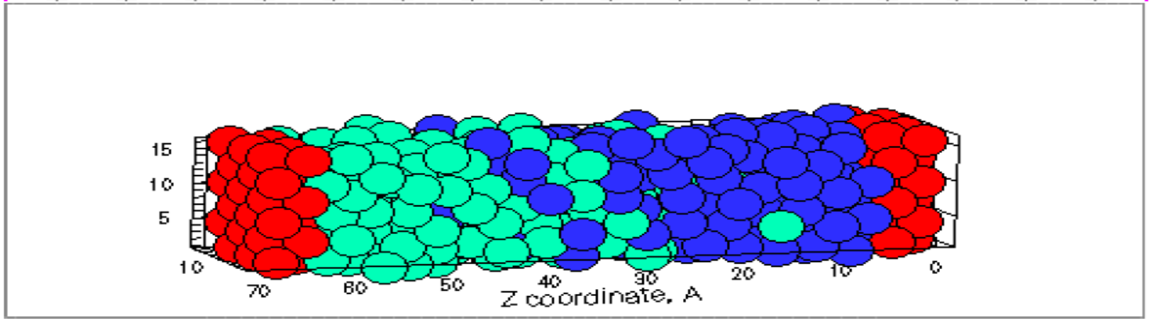
- **Factors that influence diffusion**
  - **Diffusing species**
  - **Host solid**
  - **Temperature**
  - **Microstructure**

Introduction To Materials Science, Chapter 5, Diffusion

What is diffusion?

Diffusion is material transport by atomic motion.

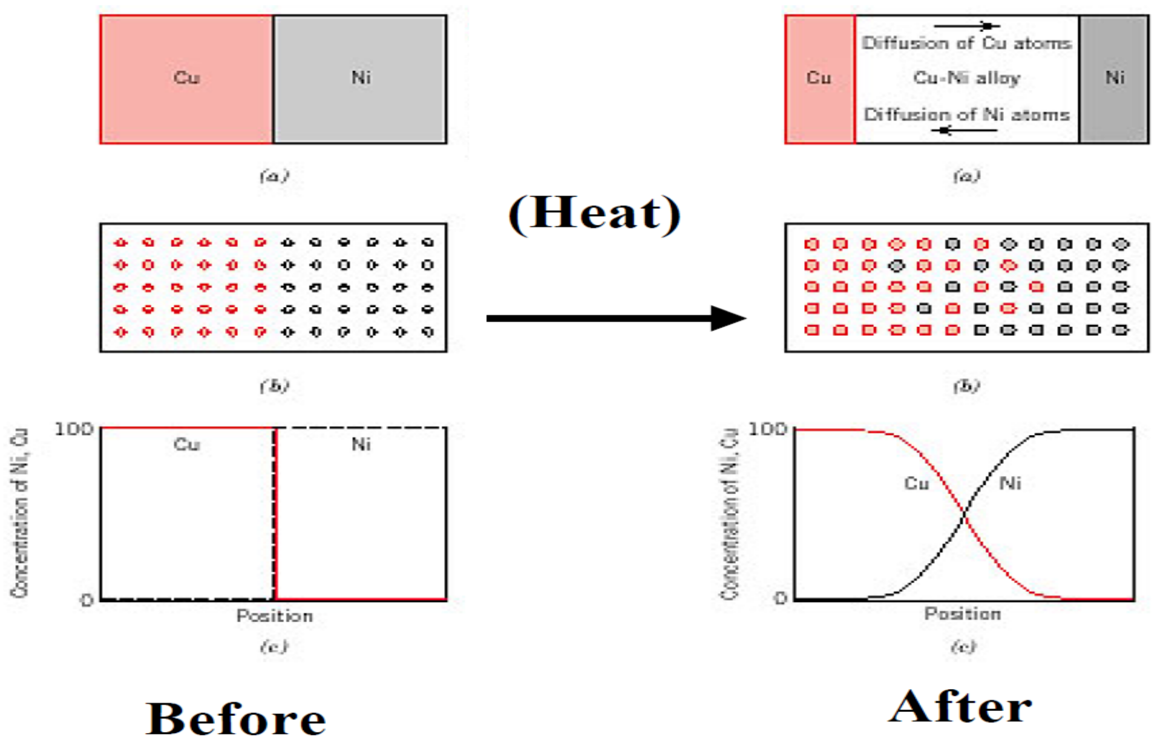




Inhomogeneous materials can become homogeneous by diffusion. For an active diffusion to occur, the temperature should be high enough to overcome energy barriers to atomic motion.

Interdiffusion and Self-diffusion

Interdiffusion (or impurity diffusion) occurs in response to a **concentration gradient**.



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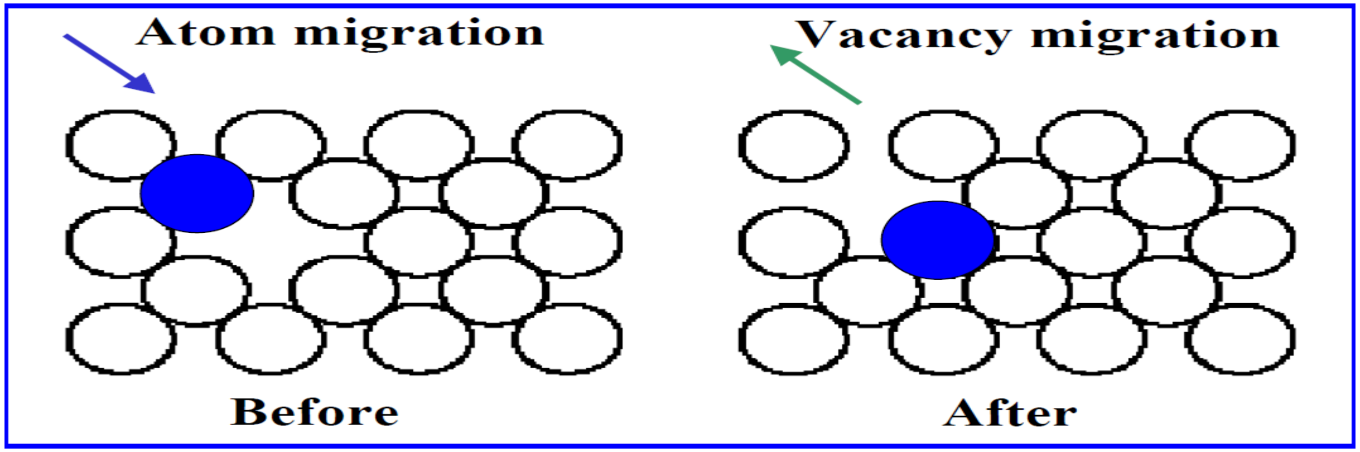
Diffusion Mechanisms (I)

Vacancy diffusion

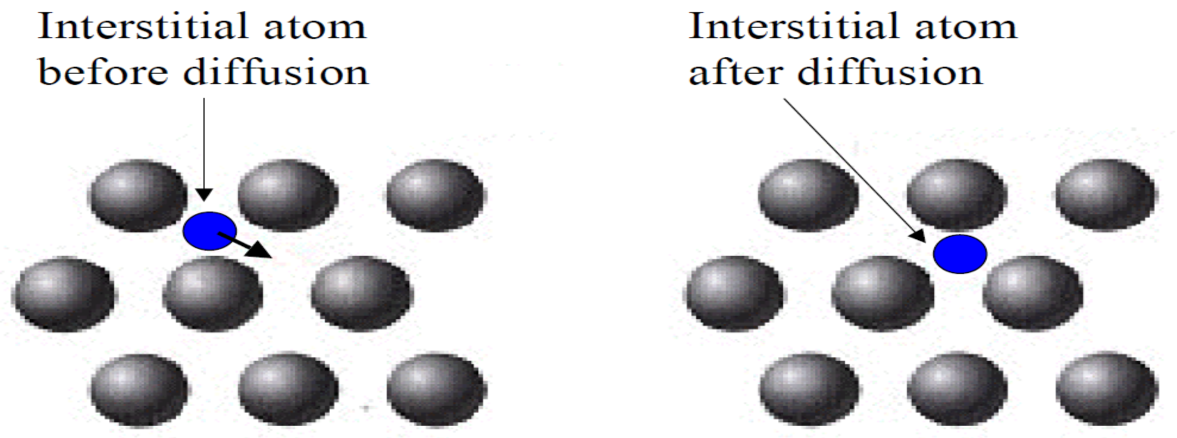


To jump from lattice site to lattice site, atoms need energy to break bonds with neighbors, and to cause the necessary lattice distortions during jump. This energy comes from the thermal energy of atomic vibrations ($E_{av} \sim kT$)

Materials flow (the atom) is opposite the vacancy flow direction.

Diffusion Mechanisms (II)

Interstitial diffusion



Interstitial diffusion is generally faster than vacancy diffusion because bonding of interstitials to the surrounding atoms is normally weaker and there are many more interstitial sites than vacancy sites to jump to.

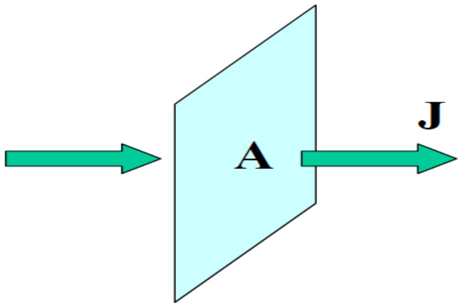
Requires small impurity atoms (e.g. C, H, O) to fit into interstices in host.

Diffusion Flux

The flux of diffusing atoms, J, is used to quantify how fast diffusion occurs. The flux is defined as either in number of atoms diffusing through unit area and per unit time (e.g., atoms/m^2-second) or in terms of the mass flux - mass of atoms diffusing through unit area per unit time, (e.g., kg/m^2-second).

$$\mathbf{J = M / At \cong (1/A)\,(dM/dt)}\ (\mathrm{Kg\ m^{-2}\ s^{-1}})$$

where M is the mass of atoms diffusing through the area A during time t.



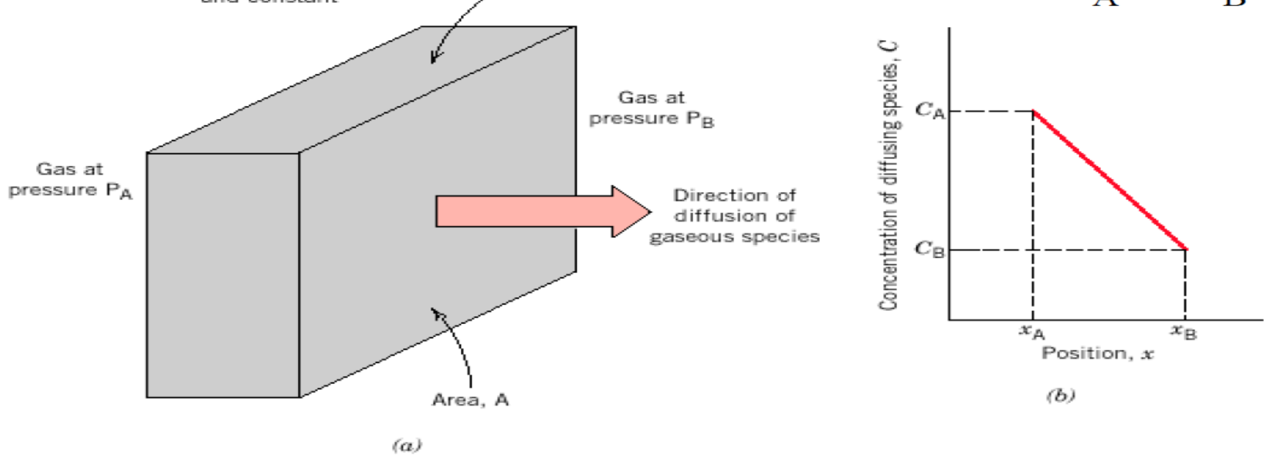
Steady-State Diffusion

Steady state diffusion: the diffusion flux does not change with time.

Concentration profile: concentration of atoms/molecules of interest as function of position in the sample.

Concentration gradient: dC/dx ($Kg.m^{-3}$): the slope at a particular point on concentration profile.

$$\frac{dC}{dx} \cong \frac{\Delta C}{\Delta x} = \frac{C_A - C_B}{x_A - x_B}$$



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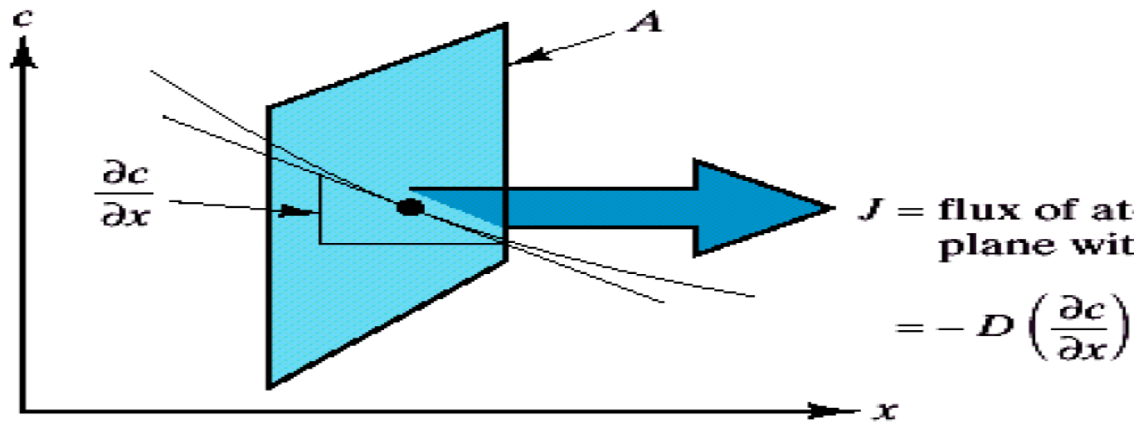
Steady-State Diffusion: Fick's first law

Fick's first law: the diffusion flux along direction x is proportional to the concentration gradient

$$J = -D\frac{dC}{dx}$$ where **D is the diffusion coefficient**



The concentration gradient is often called the *driving force* in diffusion (but it is not a force in the mechanistic sense).

The minus sign in the equation means that diffusion is down the concentration gradient.