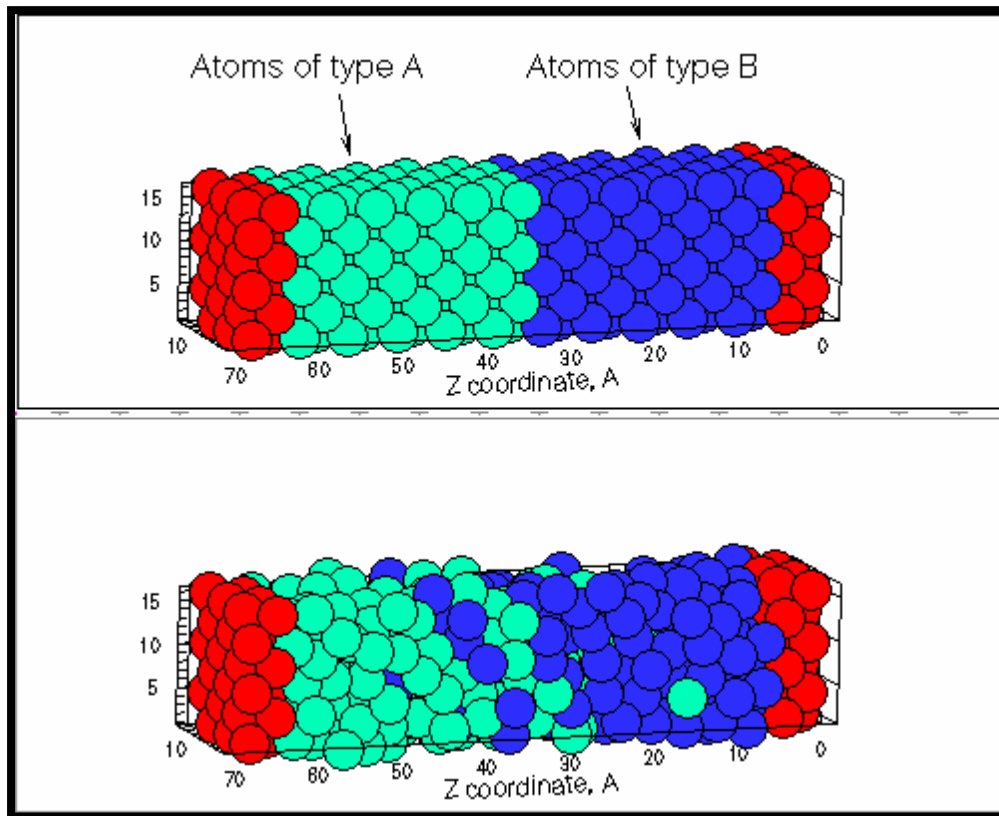


Diffusion

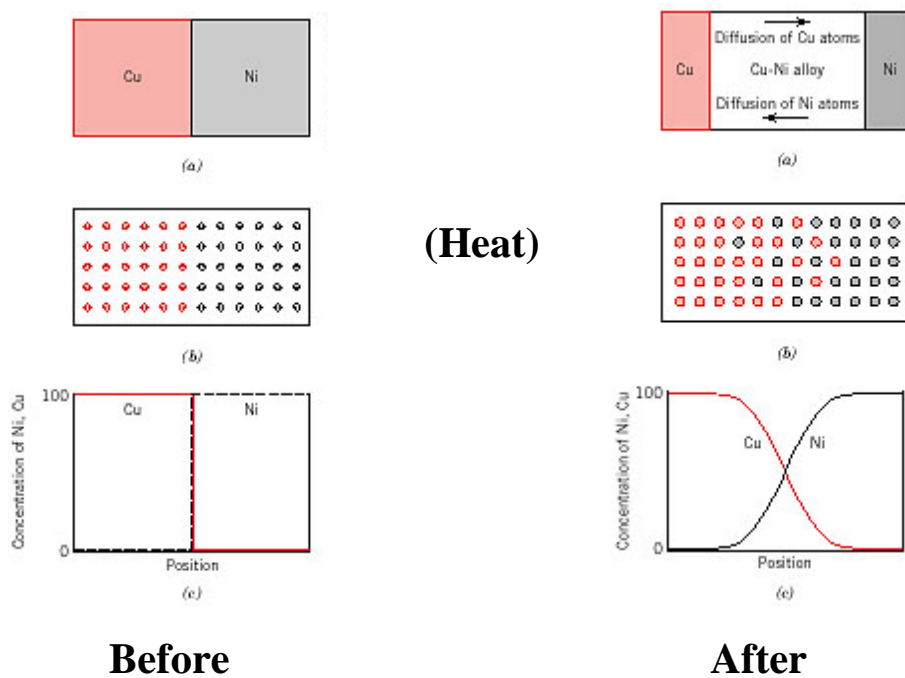
- Diffusion is material transport by atomic motion.



- 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

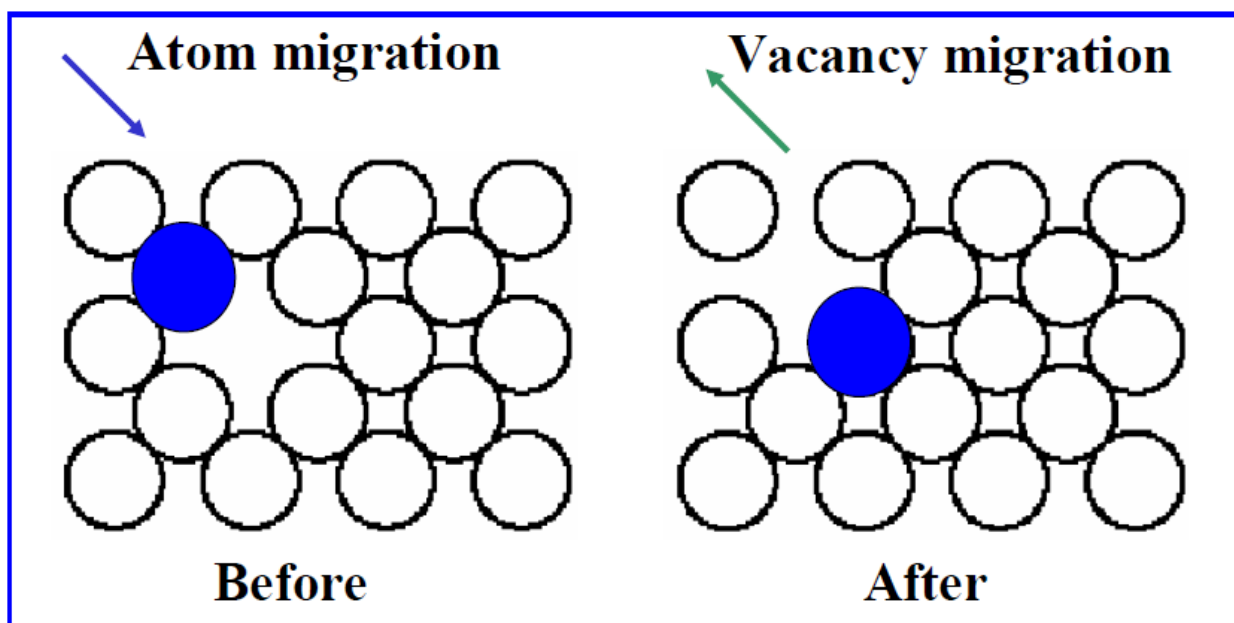
Interdiffusion (or impurity diffusion) occurs in response to a concentration gradient.



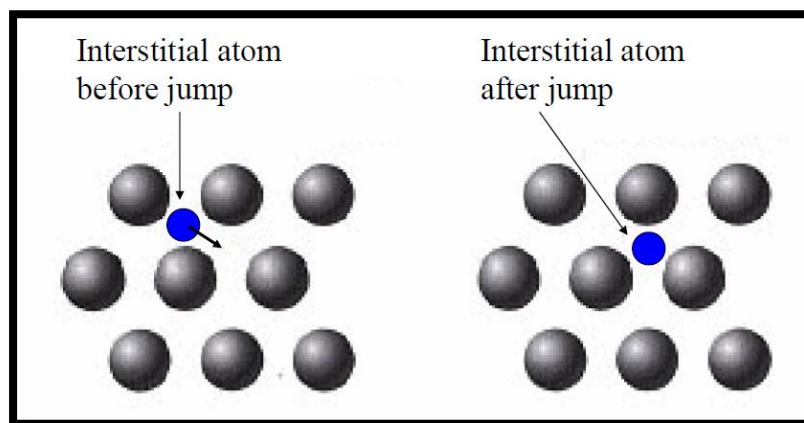
Self-diffusion is diffusion in one-component material, when all atoms that exchange positions are of the same type.

Diffusion Mechanisms

Vacancy diffusion mechanism:



- 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 ($E_{av} \sim k_B T$)
- The direction of flow of atoms is opposite the vacancy flow direction.

Interstitial diffusion mechanism:

- 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

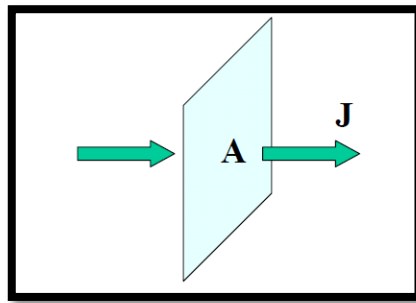
The flux of diffusing atoms, J , is used to quantify how fast diffusion occurs.

The flux is defined as either the number of atoms diffusing through unit area per unit time (atoms/m²-second) or the mass of atoms diffusing through unit area per unit time, (kg/m²- second).

For example, for the mass flux we can write:

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

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



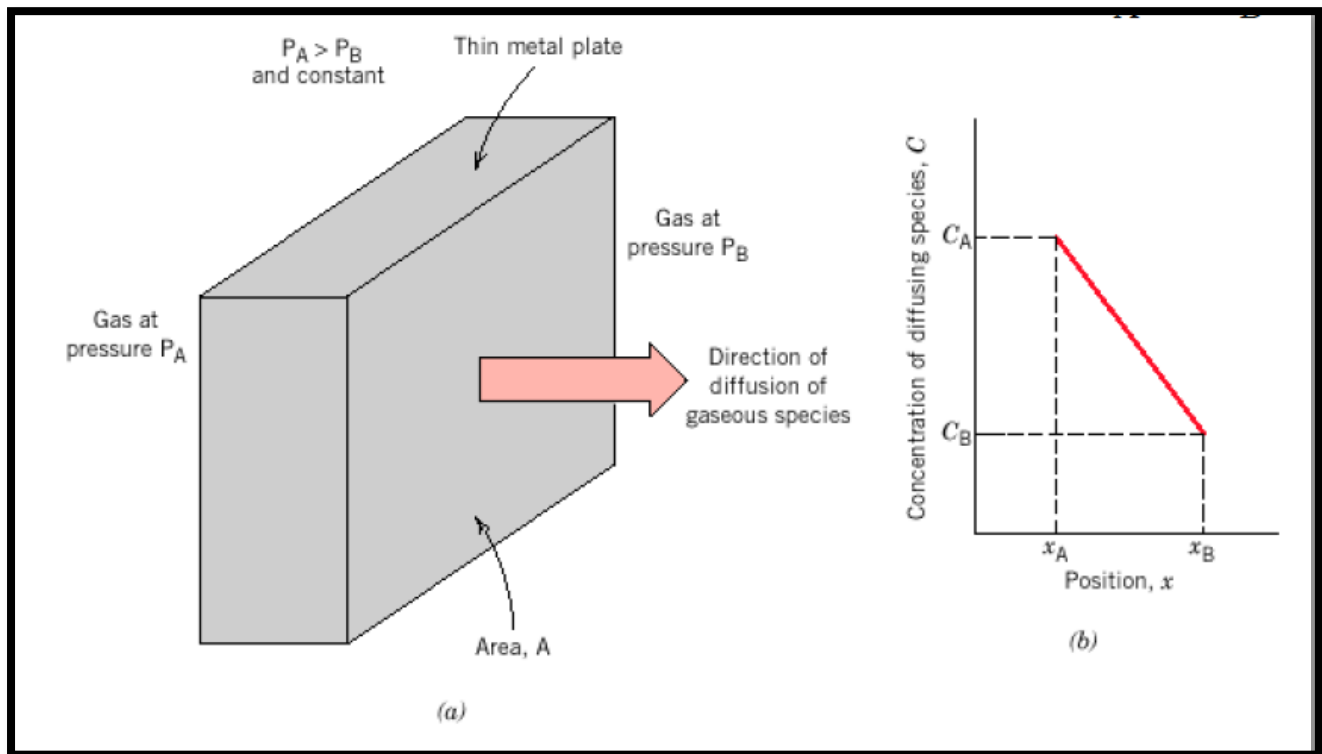
Steady-State Diffusion

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: $\mathbf{dC/dx}$ (Kg m^{-4}): the slope at a particular point on concentration profile.

$$\frac{\mathbf{dC}}{\mathbf{dx}} \cong \frac{\Delta \mathbf{C}}{\Delta \mathbf{x}} = \frac{\mathbf{C}_A - \mathbf{C}_B}{\mathbf{x}_A - \mathbf{x}_B}$$

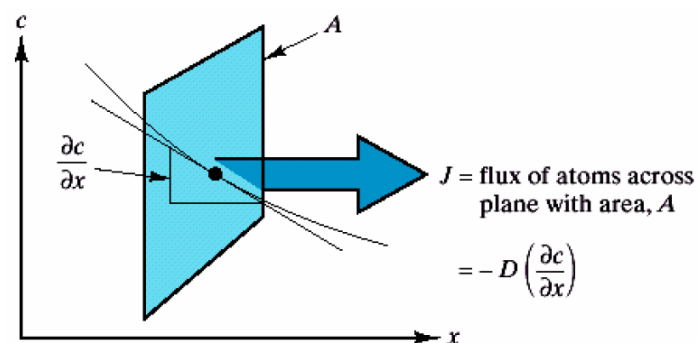


Steady-State Diffusion: Fick's first law

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.

Temperature dependence: Interstitial and vacancy diffusion mechanisms

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

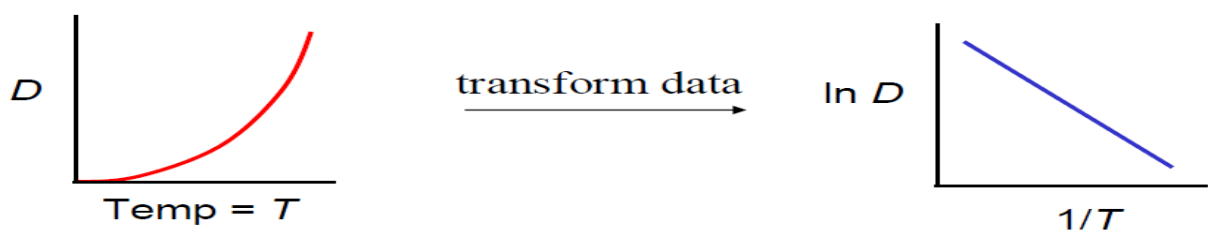
Example

At 300°C the diffusion coefficient and activation energy for Cu in Si are

$$D(300^\circ\text{C}) = 7.8 \times 10^{-11} \text{ m}^2/\text{s}$$

$$Q_d = 41.5 \text{ kJ/mol}$$

What is the diffusion coefficient at 350°C?



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

$$\ln D = \ln D_0 - \frac{Q_d}{R} \left(\frac{1}{T}\right)$$

$$\ln D_2 = \ln D_0 - \frac{Q_d}{R} \left(\frac{1}{T_2}\right) \quad \text{and} \quad \ln D_1 = \ln D_0 - \frac{Q_d}{R} \left(\frac{1}{T_1}\right)$$

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

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

$$D_2 = D_1 \exp \left[-\frac{Q_d}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) \right]$$

$$T_1 = 273 + 300 = 573 \text{ K}$$

$$T_2 = 273 + 350 = 623 \text{ K}$$

$$D_2 = (7.8 \times 10^{-11} \text{ m}^2/\text{s}) \exp \left[\frac{-41,500 \text{ J/mol}}{8.314 \text{ J/mol} \cdot \text{K}} \left(\frac{1}{623 \text{ K}} - \frac{1}{573 \text{ K}} \right) \right]$$

$$D_2 = 15.7 \times 10^{-11} \text{ m}^2/\text{s}$$