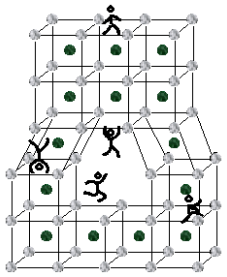
Diffusion



- Diffusion
  - Hopping
  - Concentration Gradients
- Fick's First Law of Diffusion
- Fick's Second Law of Diffusion
  - Thin Film Solution
  - Semi-infinite Solution
- Diffusion Mechanisms

MATS275: INTRODUCTION TO MATERIALS SCIENCE

Flux Equations

General Flux Equation:

Flux = (conductivity) * (driving force)

Fourier's Law (heat flow): $J_n = -\kappa \frac{dT}{dx}$

Ohm's Law (electricity): $J_e = -\sigma \frac{dV}{dx}$

Fick's First Law (diffusion): $J_D = -D \frac{dC}{dx}$

Gradient?

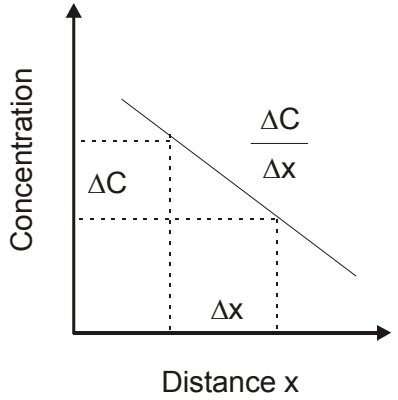
High Concentration **Low Concentration**

Statistically, these atoms can hop either right or left

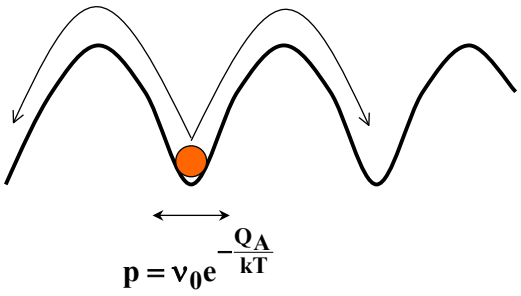
But since there are less atoms, here

The Net Flow will be to the right. This flow is called a "flux"

Concentration Profile



Atom Hopping



$$p = \nu_0 e^{-\frac{Q_A}{kT}}$$

Equally likely to hop either direction

Fick's First Law

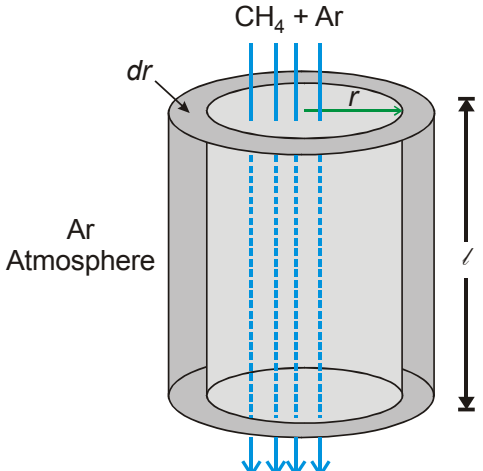
- The diffusive flux is proportional to the concentration gradient...

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

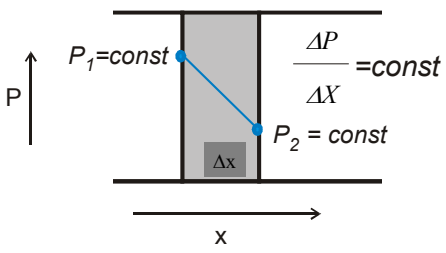
$$D = D_0 e^{-\frac{E_A}{kT}}$$

D is dependent on the host material, the diffusing species, the temperature, and the mechanism (units cm^2 / s)

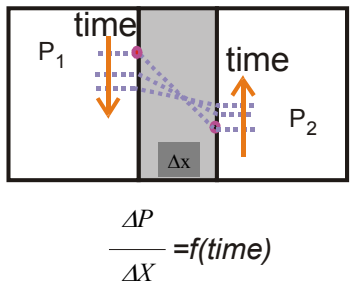
Example of Fick's First Law: Carburization



Non-Steady State Diffusion



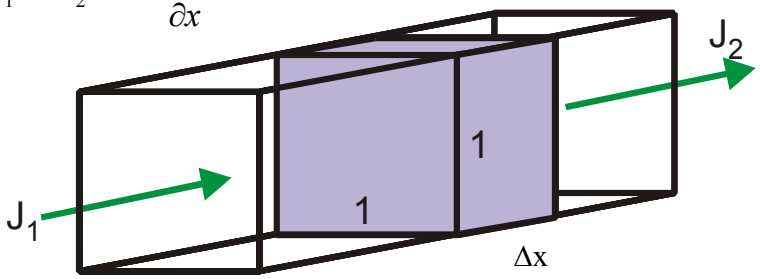
Steady State



Non-Steady State

Model for Diffusion Into a Bar

$$J_1 = J_2 - \Delta x \frac{\partial J}{\partial x}$$



(flux in = flux out – change in flux in volume element)

In Any Instant…Fick's 1st Law is Still Valid

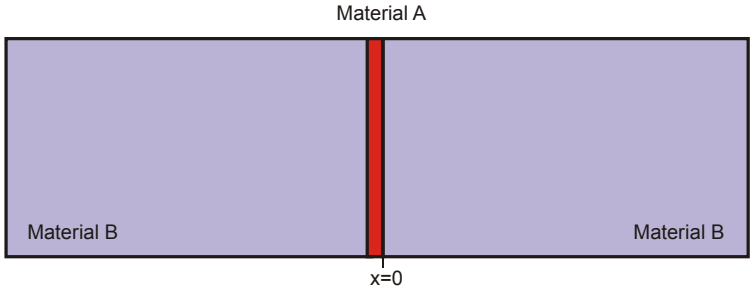
Fick's First Law: $\mathbf{J = -D\frac{dC}{dx}}$ (instantaneously)

$$\frac{\partial C}{\partial t} = -\frac{\partial J}{\partial x} \qquad \frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right)$$

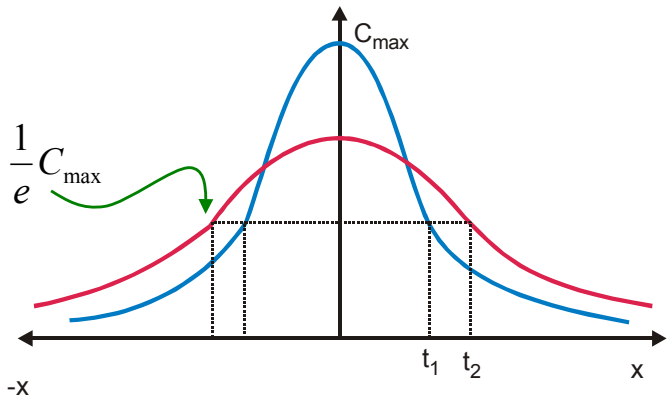
If D does not vary as a function of spatial distance (generally true), then:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$ Fick's Second Law

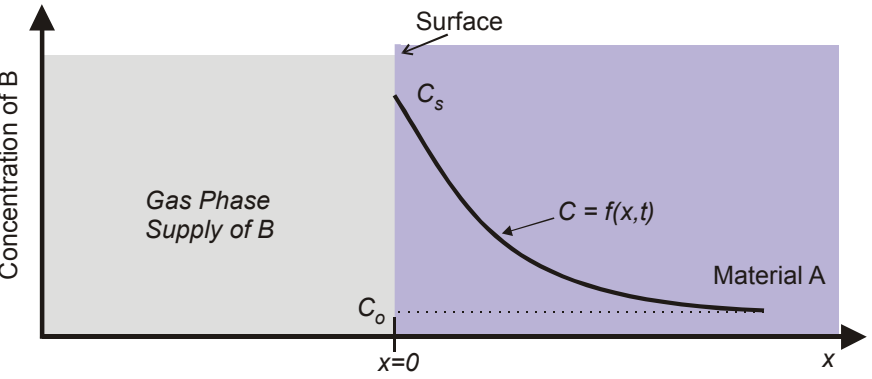
Case I: Thin Film Solution



Concentration Profile



Case II: Semi-Infinite Solid Solution



It can be shown…

$$C(x,t) = \frac{C_x - C_0}{C_s - C_0} = \left[1 - erf\left(\frac{x}{2\sqrt{DT}}\right)\right]$$

Gaussian Error Function:

$$erf(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-y^2}\, dy$$

Semiconductor Doping, $C_0 = 0$

The concentration dependence is then simplified:

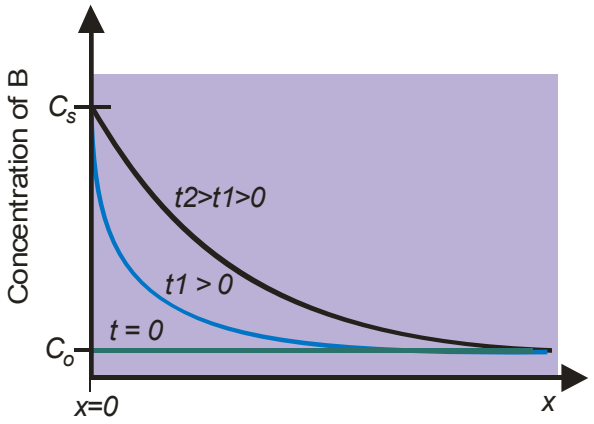
$$C(x,t) = C_S\left[1 - erf\left(\frac{x}{2\sqrt{Dt}}\right)\right]$$

Note that this is simplified to using the complimentary error function:

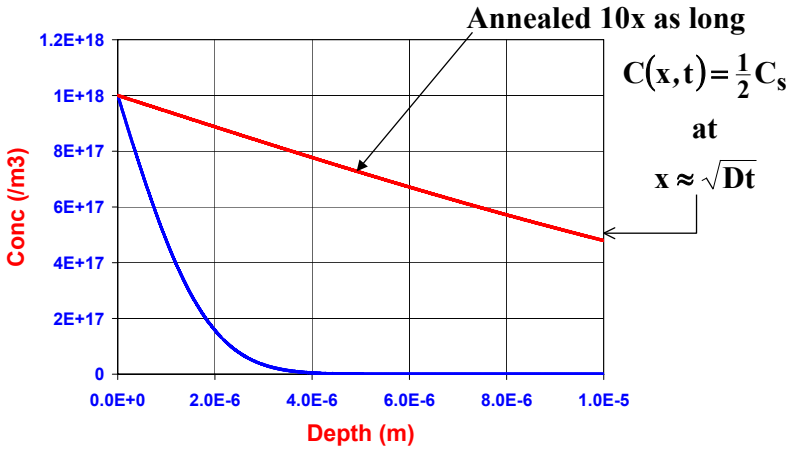
$$\frac{C_X}{C_S} = erfc\left(\frac{x}{2\sqrt{Dt}}\right) = \kappa$$

Where κ is a constant at a given instant in time.

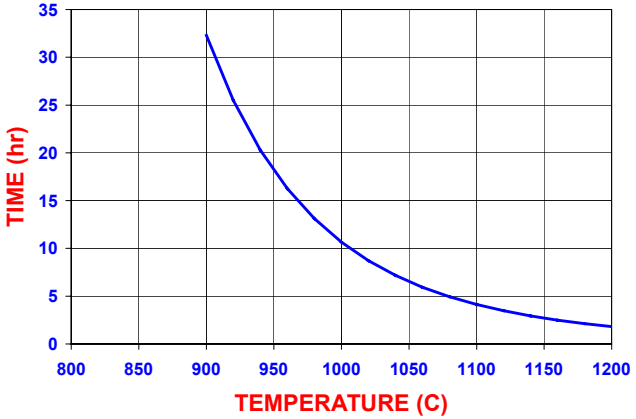
Concentration Profile



Time Dependence

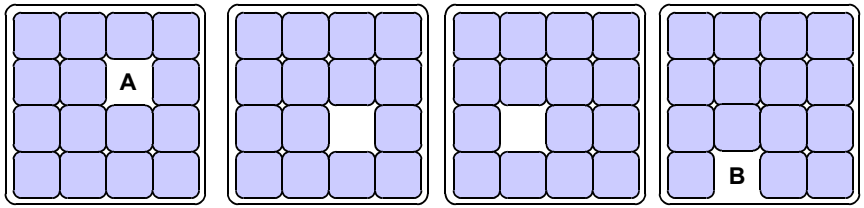


Carburizing Steel

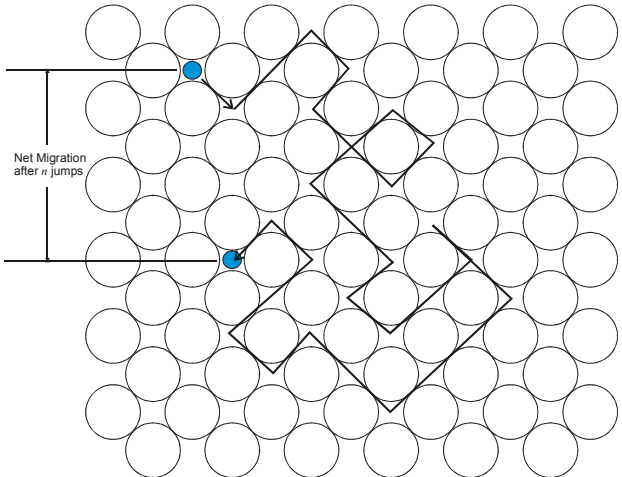


T	t
950°C	18.7h
1000°C	11.0h
1100°C	4.3h
1200°C	1.9h

Vacancy Diffusion



Interstitial Diffusion



Mechanisms

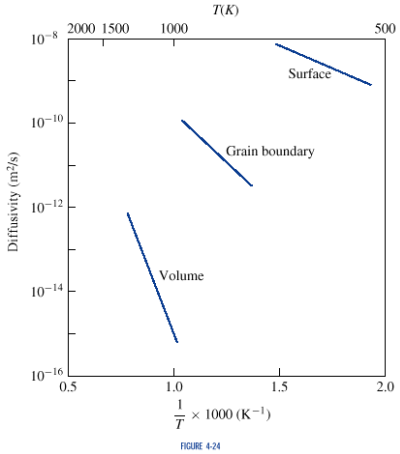
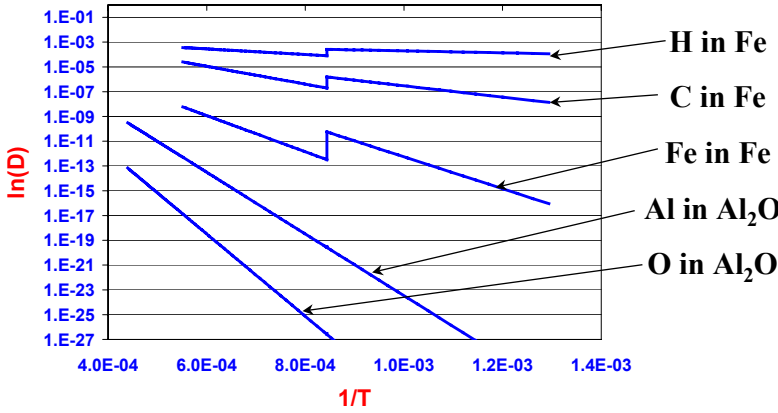


FIGURE 4-24

T Dependence of D



Activation Energy vs. Melting Point