

# MSE200

## Lecture 6 (CH. 5.1-5.4)

### Diffusion

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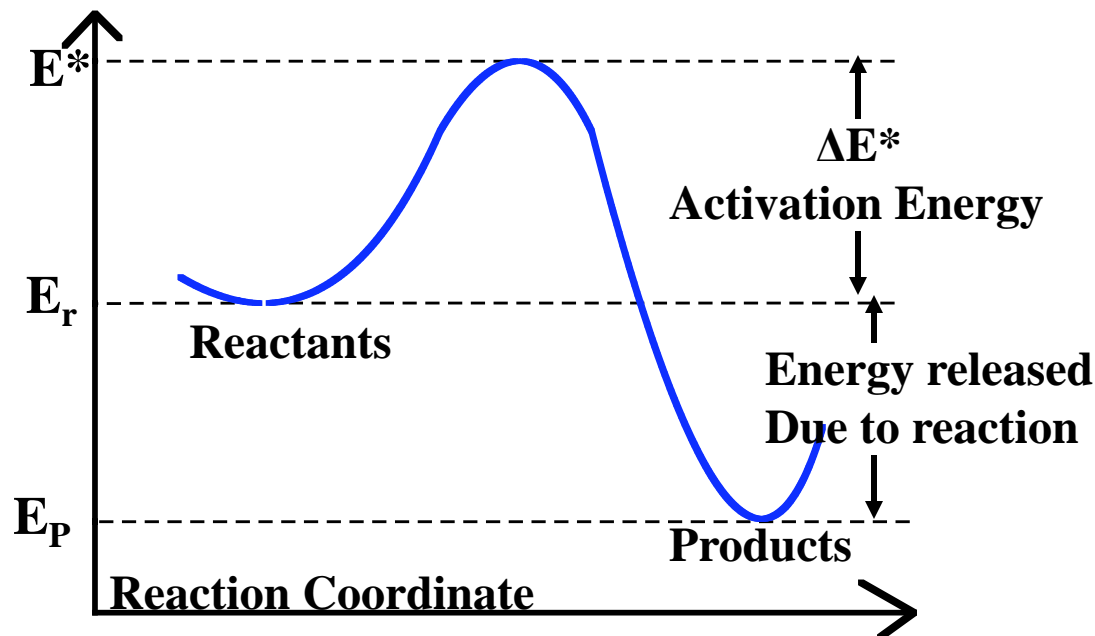
•**Objectives/outcomes: You will learn the following:**

- Describe the rate processes in solids, the activation energy.
- Describe atomic diffusion and diffusion mechanisms.
- Describe substitutional and interstitial diffusion.
- Describe steady state diffusion and apply Fick's first law.
- Describe transient diffusion and apply Fick's second law.
- Describe effect of temperature on diffusion rate.
- List a few industrial applications of diffusion.

## Rate Process in Solids

- At a given temperature, not all atoms have activation energy  $\Delta E^*$ . It should be supplied to them.

$$rate = Ce^{\frac{-\Delta E_a}{kT}} = Ce^{\frac{-\Delta E}{RT}}$$



$\Delta E^*$  = Activation Energy  
 $k$  = Boltzmann's constant  
 $= 1.38 \times 10^{-23} \text{ J/(atom K)}$

$R = 8.314 \text{ J/(mol K)}$

## Vacancy concentration

- The number of **vacancies** at equilibrium at a particular temperature in a metallic crystal lattice is given by

$$C_V = \frac{n_v}{N} = C e^{\frac{-E_v}{kT}}$$

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$n_v$  = Number of vacancies per  $m^3$  of metal

$N$  = Number of atoms per  $m^3$  of metal

$E_v$  = Activation Energy to form a vacancy

$T$  = Absolute Temperature.

$K$  = Boltzmann's Constant =  $1.38 \times 10^{-23}$  J/(atom K).

$C$  = Constant

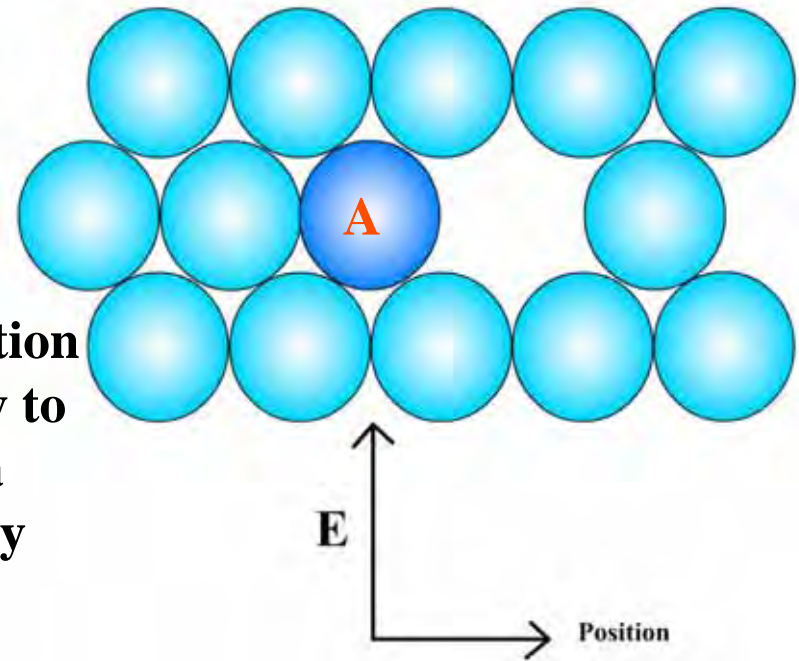
# Atomic Diffusion in Solids

- **Diffusion is a process by which a matter is transported through another matter or itself (self diffusion).**
- **Examples:**

<http://www.youtube.com/watch?v=y0WoJ3SGRck>

## Vacancy or Substitutional Diffusion

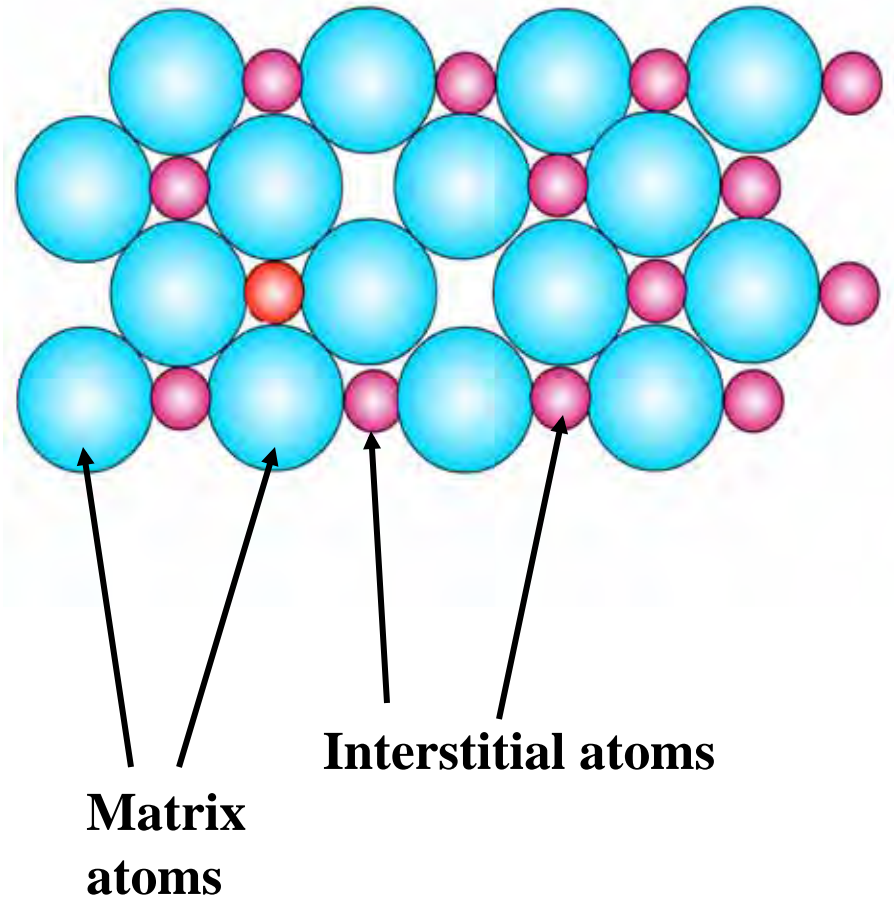
$$\text{Activation Energy of Self diffusion} = \text{Activation Energy to form a Vacancy} + \text{Activation Energy to move a vacancy}$$



- requirement: Vacancy
- As the melting point increases, activation energy also increases (why?)

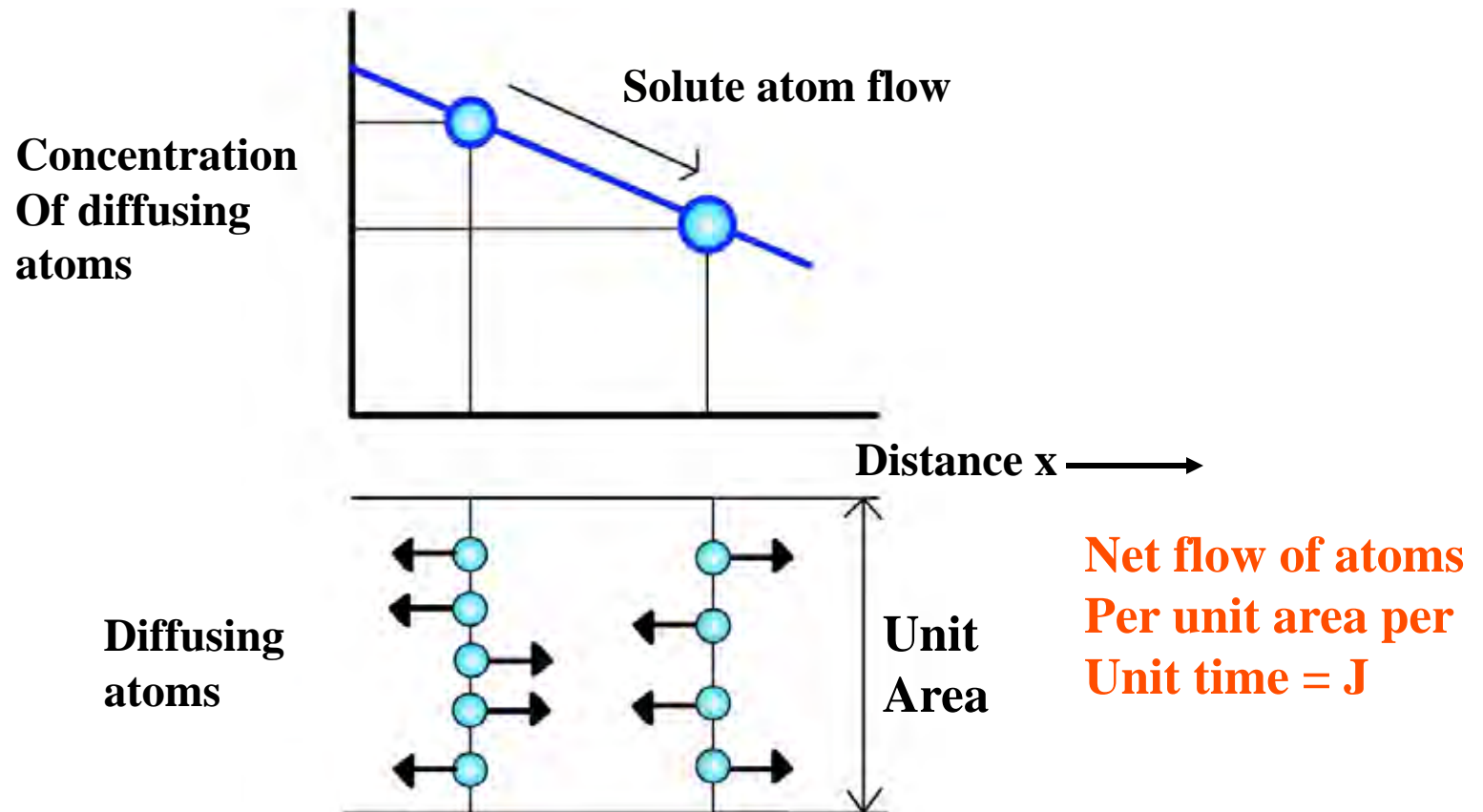
## Interstitial Diffusion mechanism

- Atoms move from one interstitial site to another.



# Steady State Diffusion

- No change in concentration with time
- No chemical reaction occurs. Only net flow of atoms.



## Fick's First Law (for steady state diffusion)

- **The flux or flow of atoms is given by**

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

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**J = Flux or net flow of atoms.**

**D = Diffusion coefficient/diffusivity**

$\frac{dc}{dx}$  = **Concentration Gradient.**

- **Temperature effect:**

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

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## Non-Steady State Diffusion

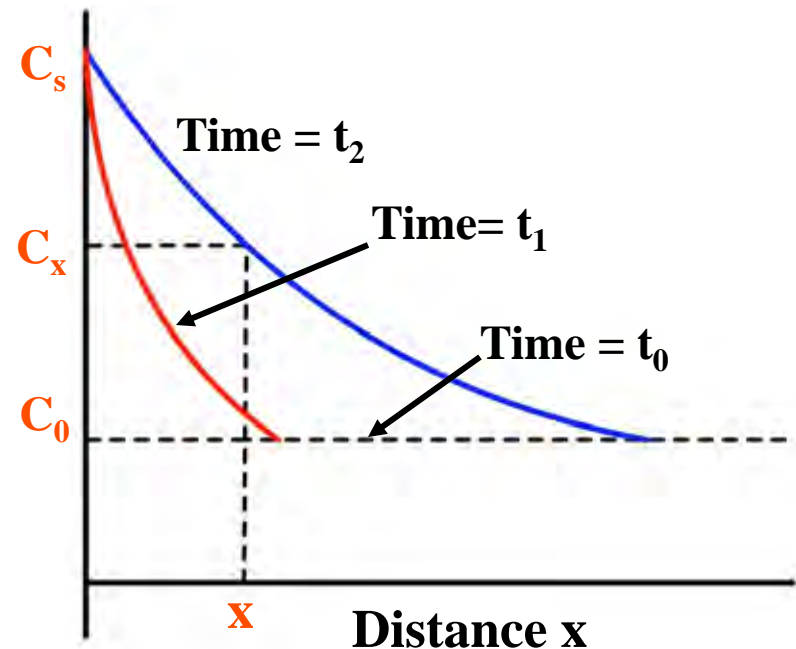
- Concentration of solute atoms at any point in metal changes with time in this case.
- **Ficks second law:**

$$\frac{dC_x}{dt} = \frac{d}{dx} \left( D \frac{dc_x}{dx} \right)$$

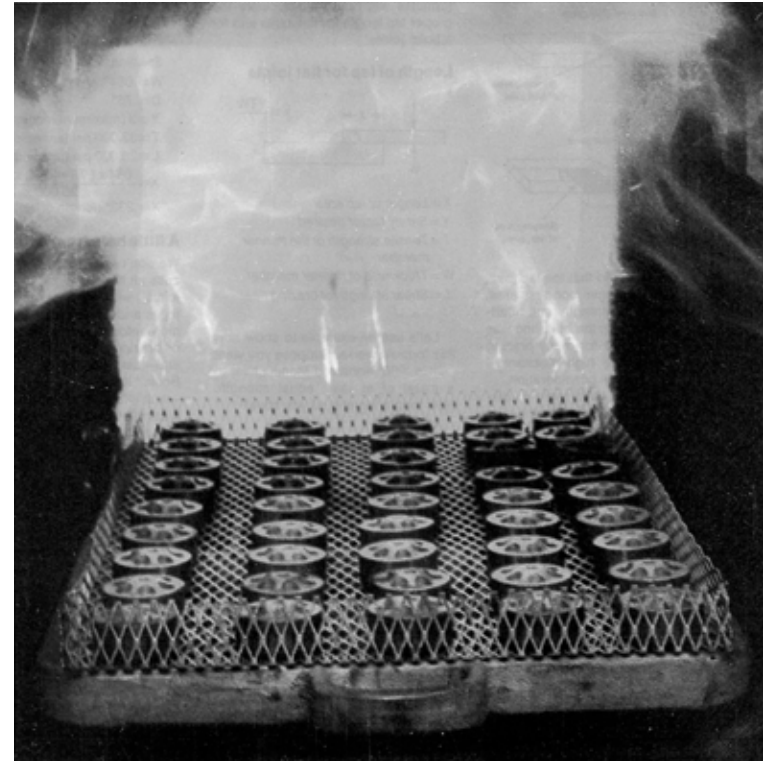
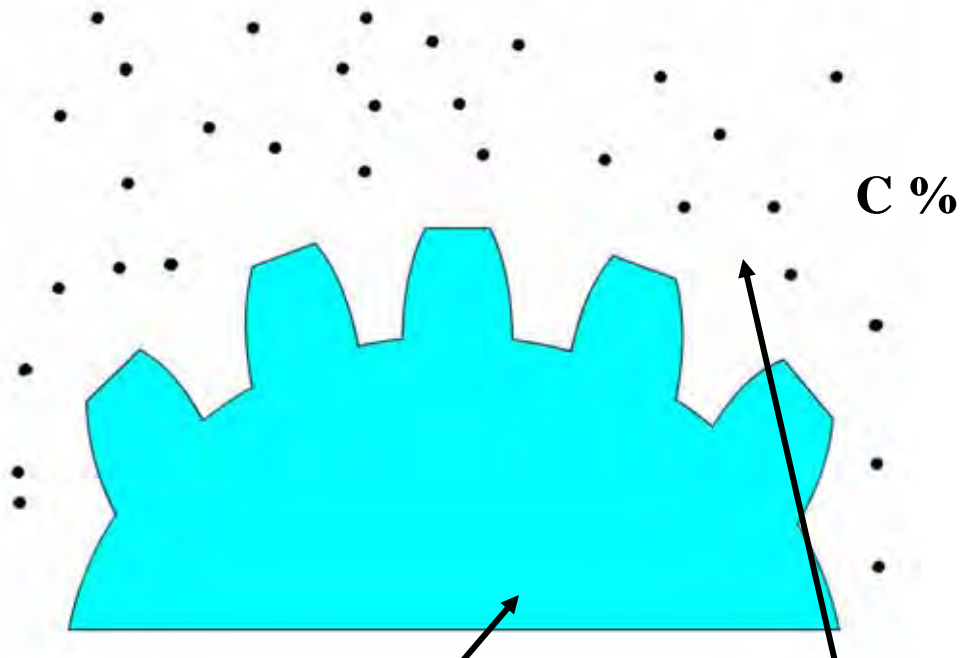
## Fick's Second Law – Solution

$$\frac{C_s - C_x}{C_s - C_0} = \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

- $C_s$  = Surface concentration of element in gas diffusing into the surface.
- $C_0$  = Initial uniform concentration of element in solid.
- $C_x$  = Concentration of element at distance  $x$  from surface at time  $t_1$ .
- $x$  = distance from surface
- $D$  = diffusivity of solute
- $t$  = time.



# Carburizing



**Low carbon  
Steel part**

**Diffusing carbon  
atoms**

## Effect of Temperature on Diffusion

- **Dependence of rate of diffusion on temperature is given by**

$$D = D_0 e^{\frac{-Q}{RT}}$$

or

$$\ln D = \ln D_0 - \frac{Q}{RT}$$

**D = Diffusivity m<sup>2</sup>/S**

**D<sub>0</sub> = Proportionality constant m<sup>2</sup>/S**

**Q = Activation energy of diffusing species J/mol**

**R = Molar gas constant = 8.314 J/mol.K**

**T = Temperature (K)**

## Effect of Temperature on Diffusion-Example

- If diffusivity at two temperatures are determined, two equations can be solved for **Q and D<sub>0</sub>**
- **Example:-**

The diffusivity of silver atoms in silver is  $1 \times 10^{-17}$  at  $500^{\circ}\text{C}$  and  $7 \times 10^{-13}$  at  $1000^{\circ}\text{C}$ .

Therefore, 
$$\frac{D_{1000}}{D_{500}} = \frac{\exp(-Q / RT_2)}{\exp(-Q / RT_1)} = \exp\left(\frac{-Q}{R} \left(\frac{1}{T_2} - \frac{1}{T_1}\right)\right)$$

$$\frac{7 \times 10^{-13}}{1 \times 10^{-17}} = \exp\left(-\frac{Q}{R} \left(\frac{1}{1273} - \frac{1}{773}\right)\right)$$

Solving for **activation energy Q**

$$Q = 183\text{KJ} / \text{mol}$$

# Home work

Example Problems: 5.1, 5.2, 5.3, 5.4, 5.5, 5.6,  
Regular Problems, Chapter 5:3, 13, 16, 21, 25,  
Reading assignment for the next class after test 1: 5.1-5.4

## Test 1 review and policy

- Understand the underlined concept in the VG
- Example problems
- Homework problems
  
- 35 multiple choices at 3 points each
- Bring your student ID
- Have you ID # for the score sheet!