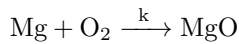


Lecture 13

1 Thermal Activation At The Atomic Scale

$$rate = Ce^{\frac{-q}{kt}} \quad (1)$$

1. $q = Q/N_{AV}$: The activation energy of per atomic scale, J or eV
2. $k = R/N_{AV}$: Boltzmann's Constant, $13.81 \times 10^{-24} J/K$ or $82.2 \times 10^{-6} eV/K$
3. C, R, T are defined as in last equation of last lecture



$$k = Ce^{\frac{-q}{kt}}$$

$$Q = ?$$

$$300^\circ C \rightarrow T_1 = 573 K$$

$$k_{300} = Ce^{\frac{-q}{kt_1}}$$

$$600^\circ C \rightarrow T_1 = 873 K$$

$$k_{300} = Ce^{\frac{-q}{kt_1}}$$

$$\frac{k_{300}}{k_{600}} = e^{\frac{-Q}{k}(\frac{1}{T_1} - \frac{1}{T_2})}$$

$$k = 8.314 J/molh \quad (2)$$

2 Thermal Production of different point Defects

$$\frac{n_{defects}}{n_{sites}} = Ce^{-\frac{E_{defect}}{kT}} \quad (3)$$

Example 5.2

$$\frac{n_v}{n_{sites}} = CCe^{-\frac{E_v}{kT}}$$

$$T_1 = 600^\circ C = 873 K$$

$$T_2 = 660^\circ C = 933 K$$

$$\frac{\frac{n_v}{n_s} 660}{\frac{n_v}{n_s} 600} = e^{-\frac{E_v}{k}(\frac{1}{T_2} - \frac{1}{T_1})} \left(\frac{n_v}{n_s} \right)_{660} = 8.82 \times 10^{-4} \quad (4)$$

3 Solid-State Diffusion Models

1. Atomic Migration: Atom migration occurs in a random walk though *vacancy migration* and *interstitial migration*
2. Interdiffusion: Diffusion will occur as a result of random walk and concentration will decrease on both sides of solid material

Applications of Solid State Diffusion:

- Case Hardening or Surface Hardening: Process of hardening surface while allowing the deeper layers to remain soft (Ex. Diffusing carbon into surface of iron)
- Silicon Doping with P for *n-type* or B for *p-type* semiconductor

How do we quantify the amount or rate of diffusion?

Diffusive Flux, J: the amount of substance that will flow through and perpendicular to a unit cross-sectional area during a unit time interval:

$$J = \frac{M}{At} \quad (5)$$

- J : Diffusive Flux, kg/m^2 , mol/m^2 , or $atoms/m^2$
- M : mass diffused, kg, mols, atoms
- A : the cross-sectional area of diffusion, m^2
- t : time elapsed, seconds

In differential form:

$$J = \frac{1}{A} \frac{dM}{dt} \quad (6)$$

Measurement of diffusion flux:

- make a thin film (membrane) of cross-sectional area
- Impose a concentration gradient
- Measure the amount of atoms diffused over time

4 Flick's 1st Law

- Assumption: The diffusion flux does not change over time or a steady state condition exists
- Flux is proportional to the negative concentration gradient $= -\frac{\partial c}{\partial x}$

$$J = D \frac{\partial c}{\partial x} \quad (7)$$

5 Flick's Second Law

- Non-steady-state diffusion: The concentration of diffusing species is a function of both time and position $c = c(x, t)$

We use the following equation:

$$\frac{\partial c_x}{\partial t} = D \frac{\partial^2 c_x}{\partial x^2} \quad (8)$$

Steady-state diffusion across a thin plate:

- One common example of s.s diffusion is the diffusion of atoms of a gas through a plate of metal (or other materials) for which the concentration (or pressure) of the diffusing species of both surfaces of the plate are held constant. The concentration distribution of inside the plate becomes unchanged after a certain amount of time reaching a s.s.
- Flick's First law in s.s becomes:

$$\frac{\partial c}{\partial x} = \frac{\Delta c}{\Delta x} = \frac{c_h - c_l}{0 - x_0} = -\frac{c_h - c_l}{x_0} \quad (9)$$

Example:

$$\begin{aligned} J &= -D \frac{\partial c}{\partial x} = \frac{\Delta c}{\Delta x} \\ &= -D \frac{c_2 - c_1}{x_2 - x_1} \\ &= 6.20 \times 10^{-11} m^2/s \times \frac{0.8 - 1.2}{(10mm - 5mm) \times 10^{-3}} \\ &= 5.0 \times 10^{-9} kg/m^2s \end{aligned} \quad (10)$$