



EGN 3365

Review on Defects & Diffusion



Expectations on Chapter 4

□ Chapter 4

- Understand concepts of imperfection or defects in solid materials.
- Be able to enumerate major categories of defects, i.e., 0D defects (vacancy, interstitial and substitutional impurity atoms), 1D defects (dislocations: edge, screw, and mixed), 2D defects (surface, grain boundaries, etc.), 3D defects (voids, foreign inclusions); Be able to describe briefly the characteristics of each type of defects
- Understand that energy is needed to break bonds and create defects
- Understand practical engineering materials always contain defects; defects in solid materials are undesirable in some cases and desirable in some other cases
- Understand the effect of temperature on concentration of vacancies
- Be able to derive the relationships between composition specified in terms of volume, molar, and weight fraction for alloys and/or physical mixtures
- Understand materials microstructure can be analyzed using characterization techniques such as optical microscope, scanning electron microscope (SEM), transmission electron microscope (TEM), etc. to reveal various features at different length scale



Expectations on Chapter 5

□ Chapter 5

- Understand the concepts of diffusion - mass transport via random motion of atoms/molecules at atomic/molecular scale and self diffusion and inter-diffusion
- Understand diffusion mechanism of vacancy diffusion and interstitial diffusion
- Understand Fick's 1st law, which relates diffusion flux to concentration gradient, and the physical meaning of each of terms involved. Be able to use Fick's 1st law to derive diffusion flux, concentration gradient/profile, or diffusion coefficient if other factors are given and also explain simple phenomena.
- Understand Fick's 2nd law, which relates change of concentration with time to diffusional flux. Understand Fick's 2nd law can be analytically solved under special conditions and be able to point the assumptions being made in those derivations. Be able to use Fick's 2nd law to explain simple phenomena. Be able to use special solution provided to solve simple problems
- Understand diffusion length and be able to use it to solve simple problems
- Understand diffusion is thermally activated and diffusion coefficient changes “exponentially” with temperature. Be able to calculate diffusion activation energy or diffusion coefficient if given sufficient data
- Understand diffusion coefficient also depend on structure



Vacancy Concentration Exercise

□ As temperature T increases, how does vacancy concentration N_v typically change for typical solid state materials?

a) Increase linearly with T as $N_v = CT$

b) Decrease inversely with T as $N_v = \frac{C}{T}$

c) Increase “exponentially” with T as $N_v = C \exp\left(-\frac{Q_v}{RT}\right)$ in which Q_v is vacancy heat of formation

d) Does not change at all

c)



Solid Solubility Exercise

❑ Based on the information provided, among Ni and Cr, which metal has higher solubility in Cu?

Ni has higher solubility in Cu

Hume-Rothery Rule for solid solution formation

- Similar atom size
- Similar electronegativity
- Same crystal structure
- Similar valence

<i>Element</i>	<i>Atomic Radius (nm)</i>	<i>Crystal Structure</i>	<i>Electro-negativity</i>	<i>Valence</i>
Cu	0.1278	FCC	1.9	+2
C	0.071			
H	0.046			
O	0.060			
Ag	0.1445	FCC	1.9	+1
Al	0.1431	FCC	1.5	+3
Co	0.1253	HCP	1.8	+2
Cr	0.1249	BCC	1.6	+3
Fe	0.1241	BCC	1.8	+2
Ni	0.1246	FCC	1.8	+2
Pd	0.1376	FCC	2.2	+2
Zn	0.1332	HCP	1.6	+2

Table on p. 118, *Callister & Rethwisch 8e.*



Defect Exercise

Which of the following are point defects

1) Vacancy

2) Interstitial atom

3) Substitutional atom

4) Grain boundary

a) 1, 2, 3

b) 1, 4

c) 2, 4

d) None

a)



Diffusion Exercise (1)

□ If diffusion through a thin plate (1D diffusion) reaches steady state, meaning the flux through the plate is constant, (a) If the diffusion coefficient is assumed to be a constant, please plot the concentration profile (i.e., C vs. x), (b) Does the concentration profile change with time and explain your answer? (c) If the diffusion coefficient actually *increases* as concentration increases, please plot the concentration profile again. Please label your plots clearly and provide brief explanation. Note:

- Fick's 1st Law $J = -D \frac{\partial C}{\partial x}$
- Fick's 2nd Law $\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial C}{\partial x} \right)$



Diffusion Exercise (1)

Continued from previous

- (a) For 1D diffusion,

Given

$$J = -D \frac{\partial C}{\partial x} = \text{constant}$$

Since D is also assumed to be a constant,

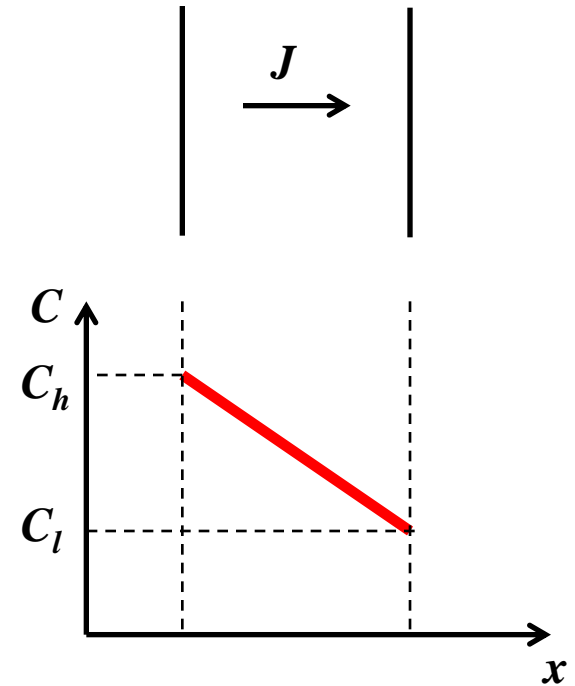
$$\text{then, } \frac{\partial C}{\partial x} = \text{constant}$$

Therefore, C vs. x is a straight line

- (b) Since diffusion flux J is constant,

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial C}{\partial x} \right) = \frac{\partial}{\partial x} (-J) = 0$$

As a result, concentration will NOT change with time





Diffusion Exercise (1)

Continued from previous

- (c) For 1D diffusion,

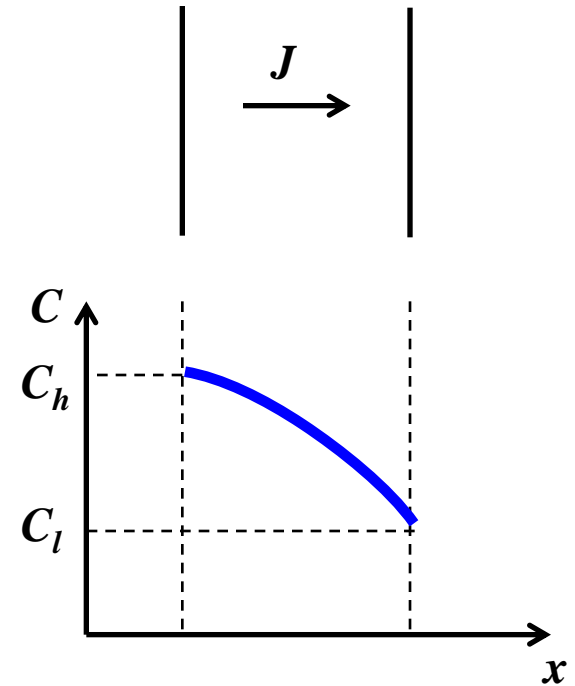
Knowing

$$J = -D \frac{\partial C}{\partial x} = \text{constant}$$

When C is higher (e.g., $C=C_h$),

to make J a constant, $\frac{\partial C}{\partial x}$ has to be smaller

Therefore, curve with curved down

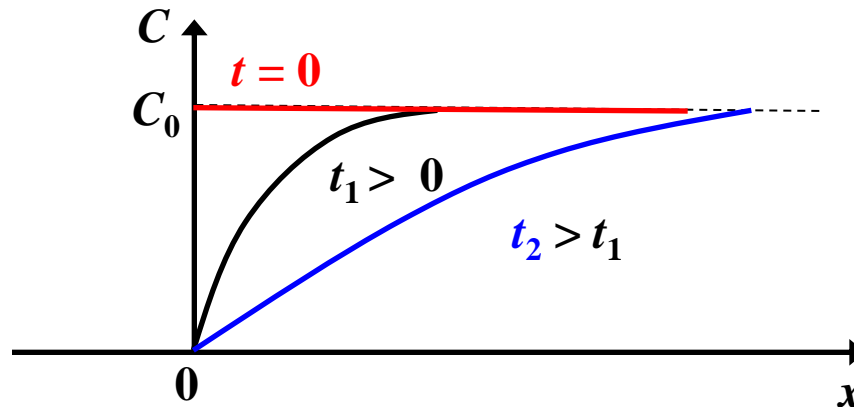




Diffusion Profile

- Sometimes, removal of carbon from surface of steel parts, or *decarburization* is carried out high temperature in vacuum. In that case, the surface concentration is kept at zero. Please sketch the change in carbon concentration profile with a steel part when it is i) before decarburization and ii) after some time t_1 and t_2 ($t_2 > t_1$) of decarburization.

Decarburization of steel





Diffusion Length Exercise (1)

- ❑ Copper is known to have damaging effect for silicon semiconductor device, knowing copper has diffusion coefficient of $2.9 \times 10^{-6} \text{ cm}^2/\text{sec}$ at $900 \text{ }^\circ\text{C}$, estimate the penetration depth for Cu atom in Si at $900 \text{ }^\circ\text{C}$ for 1 minute. Diffusion coefficient value from:

http://pearton.mse.ufl.edu/semic_properties/data/5029.pdf

Diffusion length is given by: \sqrt{Dt}

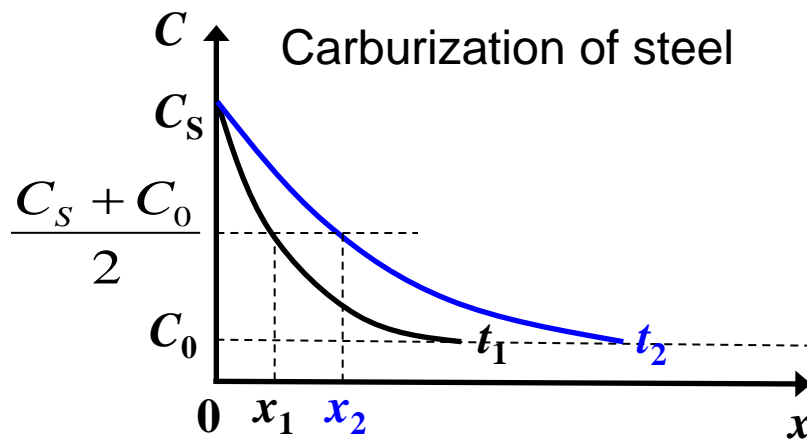
Therefore, Cu penetration depth in Si at that temperature is estimated to be:

$$\sqrt{Dt} = \sqrt{2.9 \times 10^{-6} \text{ cm}^2 / \text{sec} \times 60 \text{ sec}} = 0.013 \text{ cm} = 130 \mu\text{m}$$



Diffusion Length Exercise (2)

- When drive carbon into surface of steel by diffusion process, suppose surface carbon concentration of C_s and bulk carbon concentration of C_0 are maintained constant. Knowing at time t_1 , at depth x_1 below the surface, the carbon concentration reaches $(C_s + C_0)/2$. In order to increase the thickness of surface layer with carbon concentration at or above $(C_s + C_0)/2$ from x_1 to $x_2 = 2x_1$ please determine the time of diffusion required to achieve that.



Diffusion length

$$x_1 = \sqrt{Dt_1} \quad x_2 = 2x_1$$
$$x_2 = \sqrt{Dt_2}$$

Therefore, time required:

$$\sqrt{t_2} = 2\sqrt{t_1} \quad t_2 = 4t_1$$