

Lecture 14

1 Diffusion into semi-finite solids

Diffusion into a solid that has a finite face and an infinite body.

The solution for this is:

$$\frac{c_x - c_0}{c_s - c_0} = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \quad (1)$$

Where:

1. t is the diffusion time
2. x is the position
3. c_x the concentration of the diffusing species
4. c_s surface concentration of diffusing species
5. c_0 the initial bulk concentration

Example 5.4:

$$\begin{aligned} c_x &= 0.6\% \\ c_0 &= 0.2\% \\ c_s &= 1.0\% \\ X &= 1\text{mm} \\ \frac{c_x - c_0}{c_s - c_0} &= 0.5 \\ D &= 2.98 \times 10^{-11} \frac{\text{m}^2}{\text{s}} \end{aligned} \quad (2)$$

$$\begin{aligned} \frac{c_x - c_0}{c_s - c_0} &= 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \\ \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) &= 1 - \frac{c_x - c_0}{c_s - c_0} \\ &= 0.5 \\ t &= 3.68 \times 10^4 \text{s} \end{aligned} \quad (3)$$

Example 5.5:

Recalculate above with master plot:

$$\begin{aligned} \frac{c_x - c_0}{c_s - c_0} &= 0.5 \\ \Rightarrow \frac{x}{\sqrt{Dt}} &= 0.95 \\ \Rightarrow t &= 3.72 \times 10^4 \text{s} \end{aligned} \quad (4)$$

2 Diffusivity Equations

$$D = D_0 E^{-\frac{Q}{RT}} \quad (5)$$

Where:

1. D_0 preexponential constant
2. Q the activation energy per mole of diffusing species or for the motion of one diffusing species (J/mol, J, or eV)
3. R the universal gas constant

4. T the absolute temperature

In general diffusion occurs faster in BCC than in FCC structure.

We can also have diffusivity data for non-metals. Note that for non-metals the diffusivity rate is many orders of magnitude lower than that of metals.

Example 5.6:

$$\begin{aligned} D &= D_0 E^{\frac{-Q}{RT}} \\ D_0 &= 20 \times 10^{-6} \\ Q &= 1.42 \times 10^5 \\ D &=? \end{aligned} \tag{6}$$

$$\begin{aligned} \frac{c_x - c_0}{c_s - c_0} &= 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \\ \frac{0.35 - 0.20}{1 - 0.2} &= 1 - \operatorname{erf}\left(\frac{4\text{mm}}{2\sqrt{D(49.5\text{hours})}}\right) \\ \Rightarrow D &= 2.6 \times 10^{-11} \frac{m^2}{s} \\ T &= \frac{Q}{k(\ln D_0 - \ln D)} \\ &= 1260.2 \text{ K} \end{aligned} \tag{7}$$

3 Diffusion in Semiconducting Materials

We need to be able to dope our semiconductors to yield special electronic properties.

1. Pre-Deposition

- Impurity atoms (e.g. P or B) are diffused into silicon often from a gas phase. 900 °C to 1000 °C
- The concentration of the dopant in gas phase and at silicon surface are kept constant
- Semi-infinite diffusion model can be applied.

2. Drive-in Diffusion

- This treatment is used to transport atoms farther into silicon to provide more suitable concentration distribution without increasing impurity content
- Temperature is increased upto 1200 °C
- Treatment applies a SiO₂ layer to prevent escape of impurity.

4 Drive-in Diffusion

1. The impurity atoms introduced are confined to a very thin layer of the silicon
2. Then the solution to Flick's second law is:

$$C(x, t) = \frac{Q_0}{\sqrt{\pi D_d t}} e^{\frac{-x^2}{4D_d t}} \tag{8}$$

Where:

- $C(x, t)$ is the impurity concentration at position and time.
- D_d is the diffusion coefficient in the drive-in step
- Q_0 is the total amount of impurities per unit area in the solid that were introduced during the pre-deposition treatment which is:

$$Q_0 = 2C_s \sqrt{\frac{D_p t_p}{\pi}} \tag{9}$$

Where

- C_s is the surface concentration for the pre-deposition step
- D_p is the diffusion coefficient in the pre-deposition step
- t_p is the pre-deposition treatment time

Junction Depth, x_j : The Depth at which the diffusing impurity concentration is just equal to the background concentration of that impurity in the silicon.

$$x_j = \sqrt{(4D_d t_d) \ln\left(\frac{Q_0}{C_B \sqrt{\pi D_d t_d}}\right)} \quad (10)$$

Example 5.7:

a)

$$\begin{aligned} Q_0 &= 2C_s \sqrt{\frac{D_p t_p}{\pi}} = 3.44 \times 10^{18} \frac{\text{atoms}}{\text{m}^2} \\ t_p &= 30\text{mm} \times 60 \frac{\text{s}}{\text{m}} \\ C_s &= 3 \times 10^{26} \\ D_p &= D_0 e^{\frac{-q}{kT}} \\ &= 5.73 \times 10^{-20} \frac{\text{m}^2}{\text{s}} \end{aligned} \quad (11)$$

b)

$$\begin{aligned} x_j &= \sqrt{(4D_d t_d) \ln\left(\frac{Q_0}{C_B \sqrt{\pi D_d t_d}}\right)} \\ &= 2.19 \times 10^{-6} \text{m} \\ &= 2.19 \mu\text{m} \end{aligned} \quad (12)$$

$$D_d = D_0 e^{\frac{-q}{kT_d}} = 1.51 \times 10^{-17} \frac{\text{m}^2}{\text{s}} \quad (13)$$

c)

$$C(x, t) = \frac{Q_0}{\sqrt{\pi D_d t}} e^{\frac{-x^2}{4D_d t}} = 5.90 \times 10^{23} \frac{\text{atoms}}{\text{m}^3} \quad (14)$$