

Lecture 15-17:

Diffusion in solids: elementary concepts of phenomenological & atomistic approaches

Questions:

1. If iron is kept at 1200°K in a carburizing atmosphere for 8hrs to obtain a carbon concentration of 0.75 at a depth of 0.5mm. Find the time it would take to reach same carbon concentration at depth of 7.5mm at 1250°K. (Given $D_0 = 0.2 \times 10^{-4} \text{ m}^2/\text{s}$ & $Q = 143 \text{ kJ/mole/}^\circ\text{K}$)
2. A steel containing 0.2 % carbon was heated to 950°K for 15 hours. Find the depth of layer in which there is no carbide. Assume that steel consists of ferrite and carbide. The solubility of carbon in ferrite at this temperature is 0.015% and % C at the surface is negligible. (Given $D_0 = 2 \times 10^{-6} \text{ m}^2/\text{s}$ & $Q = 84.4 \text{ kJ/mole/}^\circ\text{K}$)
3. The concentration of carbon on the surface of iron is maintained at 1.00% at 1175°K for 2hours. Estimate the depth at which % C would be 0.5%. Use the diffusivity values given in question1. Assume initial carbon content of iron to be negligible.
4. Plot the concentration profile of carbon in iron sample which was kept at 927°C for 8hours while maintaining 1 % carbon concentration at its surface. Assume initial carbon content of iron as negligible.
5. It is often thought that that species having lower activation energy diffuses faster than the one having higher activation energy. Is this always true?
6. Rank the following samples in order of increasing self diffusion coefficients (a) Aluminium single crystal, (b) Polycrystalline aluminium whose average grain size is 5micron (c) Polycrystalline aluminium whose average grain size is 10micron.

Answer:

1. If iron is kept at high temperature in an environment having high carbon potential it diffuses into iron. The depth of carburization (x) is proportional to \sqrt{Dt} . Therefore $\frac{x_1}{x_2} = \sqrt{\frac{D_1 t_1}{D_2 t_2}}$ Since $D = D_0 \exp\left(-\frac{Q}{RT}\right)$ $\left(\frac{x_1}{x_2}\right)^2 = \frac{t_1}{t_2} \exp\left\{\frac{Q}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)\right\}$ Therefore $\left(\frac{0.50}{0.75}\right)^2 = \frac{8}{t} \exp\left\{\frac{143000}{8.33}\left(\frac{1}{1250} - \frac{1}{1200}\right)\right\} = 10.14 \text{ hours}$
2. If initial carbon in steel is C_i & soluble carbon in ferrite is C_α amount carbon to removed / unit cross section through a distance $dx = (C_i - C_\alpha)dx = \text{flux of carbon atom in time } dt = -Jdt = D \frac{dC}{dx} dt$ Assuming carbon concentration at surface as 0 $\frac{dC}{dx} = \frac{C_\alpha - 0}{x}$ Thus $(C_i - C_\alpha)dx = D \frac{C_\alpha}{x} dt$

or, $x = \sqrt{\frac{2DtC_a}{(C_i - C_0)}} D = D_0 \exp\left(-\frac{Q}{RT}\right) = 2 \times 10^{-6} \exp\left\{-\frac{84400}{8.31 \times 950}\right\} = 4.55 \times 10^{-11} \text{m}^2/\text{s}$ Now $C_i = 0.2$ & $C_a = 0.015$ Therefore $x = \sqrt{\frac{2 \times 4.55 \times 10^{-11} \times 0.015 \times 15 \times 3600}{(0.2 - 0.015)}} = 0.00063 \text{m} = 0.63 \text{mm}$

3. Carbon content at surface $C_s = 1.00$, Initial carbon $C_0 = 0.0$ & carbon content at a distance x $C = 0.5$

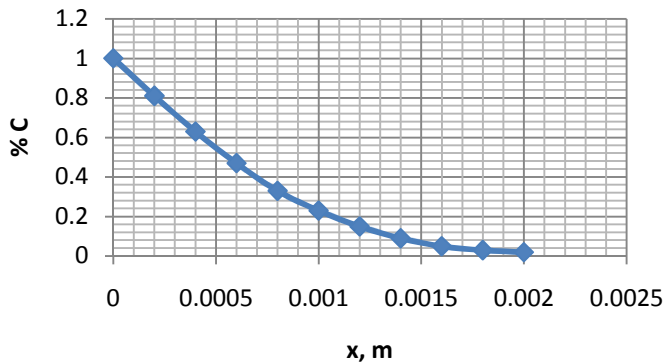
$$\frac{C_s - C}{C_s - C_0} = \text{erf}\left[\frac{x}{2\sqrt{Dt}}\right] \text{ Or, } \frac{1.0 - 0.5}{1.0} = \text{erf}\left[\frac{x}{2\sqrt{Dt}}\right] \text{ Or, } \frac{x}{2\sqrt{Dt}} = 0.477$$

$$\text{Or, } x = 0.477 \times 2 \times \sqrt{0.2 \times 10^{-4} \exp\left(-\frac{143000}{8.31 \times 1275}\right) \times 2 \times 3600} = 0.000425 \text{m} = 0.445 \text{mm}$$

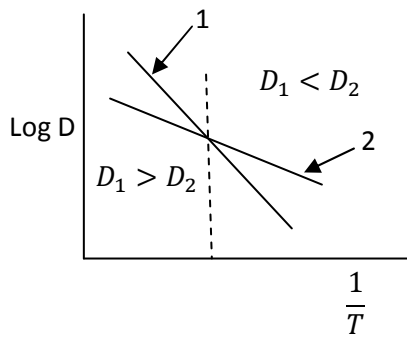
4. Carbon concentration (profile) is given by $C = C_s - C_s \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right) = 1 - \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$

| | | |
|---------------------|----------|------------------|
| D0 | 2.00E-05 | m/s ² |
| Q | 143 | kJ |
| T | 1200 | K |
| D | 1.18E-11 | m/s ² |
| t | 8 | hr |
| (Dt) ^{0.5} | 0.000584 | |

| x, m | c % |
|--------|------|
| 0 | 1.00 |
| 0.0002 | 0.81 |
| 0.0004 | 0.63 |
| 0.0006 | 0.47 |
| 0.0008 | 0.33 |
| 0.001 | 0.23 |
| 0.0012 | 0.15 |
| 0.0014 | 0.09 |
| 0.0016 | 0.05 |
| 0.0018 | 0.03 |
| 0.002 | 0.02 |



5. Assume diffusivities of two species in a given matrix are given by $D_1 = D_{01} \exp\left(-\frac{Q_1}{RT}\right)$ & $D_2 = D_{02} \exp\left(-\frac{Q_2}{RT}\right)$ respectively. Let $Q_1 > Q_2$. Let us plot logarithm of diffusivity against reciprocal of temperature. Such plots are known as Arrhenius plot whose slope gives activation energy.



This clearly shows that there might be a critical temperature shown by dotted line where both have identical diffusivity. In this case at lower temperatures species 2 has higher diffusivity whereas at higher temperature species 1 has higher diffusivity.

6. Diffusion through grain boundaries is much faster. Since single crystal does not have any grain boundary its diffusivity is the lowest. Finer the grains provide more number of high diffusivity paths. Therefore diffusivity is expected to be higher. Thus $D_a > D_c > D_b$