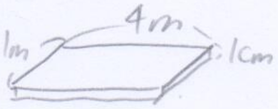
Phase transformation HW #3 20192742 손수정

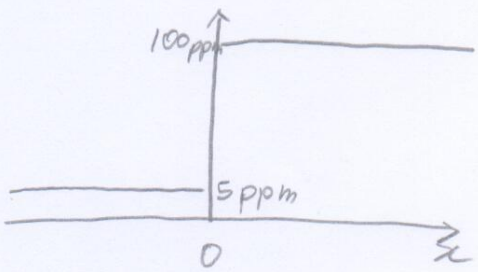
1. 

with nitrogen content of 100 ppm. (환경는 5ppm)

diffusivity of atomic nitrgen : $4 \times 10^{-7} cm^2 s^{-1}$

(a) bottom과 edge 에서의 nitrogen loss는 무시하므로. 1cm 두께 방향을 x축으로 하여 표면 $(x=0)$ 에서부터의 nitrogen loss 를 고려함.

이는 아래와 같이 표현 가능하다.



$$\frac{\partial \rho}{\partial t} = -\nabla \cdot J \quad (\text{이때 } J = -D\frac{\partial \rho}{\partial x})$$

$$= -\nabla \cdot (-D\nabla \rho) = D\nabla^2 \rho = D\frac{\partial^2 \rho}{\partial x^2} \text{ //}$$

이때 Boundary condition for $\rho(x,t)$

$$\begin{cases} \rho(x>0,0)=100 & (0 \le x < 1cm) \\ \rho(x\le 0,t)=5 \\ \rho(0,t)=5. \end{cases}$$

(b) $\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$ / $C(x,t) = \frac{A}{\sqrt{t}} \exp\left(-\frac{x^2}{4Dt}\right)$

전체 물질의 양을 M이라고 할때 $\int_{-\infty}^{\infty} C dx = M \rightarrow A = \frac{M}{\sqrt{4\pi D}}$

$$C(x,t) = \frac{M}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right)$$

이때 (a)에서 x축에 따라 plate를 무한히 나누어 i번째 film의 $\rho_i(x.t)$는

$$\rho_i(x,t) = \frac{\rho_0 \Delta a_i}{\sqrt{4\pi Dt}} \exp\left(-\frac{(x-a_i)^2}{4Dt}\right) \qquad \rho_0 = 100 \quad a_i < 0$$

$$\rho_0 = 5 \quad a_i > 0.$$

$$\rho(x.t) = \sum_i^{\infty} \rho_i = \int_0^{\infty} \frac{5}{\sqrt{4\pi Dt}} \exp\left(-\frac{(x-a_i)^2}{4Dt}\right) da$$

$$+ \int_{-1}^{0} \frac{100}{\sqrt{4\pi Dt}} \exp\left(-\frac{(x-a_i)^2}{4Dt}\right) da$$

$y = \dfrac{(x-a)}{\sqrt{4Dt}}$ 로 두면. $dy = -\dfrac{1}{\sqrt{4Dt}}\, da \qquad -\sqrt{4Dt}\, dy = da.$

$$\rho(x.t) = -\frac{5}{\sqrt{\pi}} \int_{\infty}^{\frac{x}{\sqrt{4Dt}}} e^{-y^2} dy - \frac{100}{\sqrt{\pi}} \int_{\frac{x}{\sqrt{4Dt}}}^{\frac{x-1}{\sqrt{4Dt}}} e^{-y^2} dy$$

$$= \frac{5}{\sqrt{\pi}} \left(\int_0^{\infty} e^{-y^2} dy - \int_0^{\frac{x}{\sqrt{4Dt}}} e^{-y^2} dy \right) + \frac{100}{\sqrt{\pi}} \left(\int_0^{\frac{x}{\sqrt{4Dt}}} e^{-y^2} dy - \int_0^{\frac{x-1}{\sqrt{4Dt}}} e^{-y^2} dy \right)$$

$$= \frac{5}{2} - \frac{5}{2} \mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right) + 50 \mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right) - 50 \mathrm{erf}\left(\frac{x-1}{\sqrt{4Dt}}\right)$$

(c). average nitrogen concentration $= \int_0^1 \rho(x.t)\, dx$

$$= \int_0^1 \left(-\frac{5}{2} + \frac{5}{2} \mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right) - 50 \mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right) + 50 \mathrm{erf}\left(\frac{x-1}{4Dt}\right) \right) dx$$

$$\int \mathrm{erf}(x)\, dx = x\,\mathrm{erf}(x) + \frac{e^{-x^2}}{\sqrt{x}} + C$$

$$\int \mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right) dx = x\,\mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right) + \sqrt{\frac{4Dt}{\pi}} \exp\left(-\frac{x^2}{4Dt}\right) + C$$

$$\int_0^1 \rho(x,t)\,dx = \int_0^1 \left(\frac{5}{2} - \frac{5}{2}\mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right) + 50\,\mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right) - 50\,\mathrm{erf}\left(\frac{x-1}{\sqrt{4Dt}}\right)\right)dx$$

$$= \frac{5}{2} + \frac{95}{2}\left[x\,\mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right) + \sqrt{\frac{4Dt}{\pi}}\exp\left(-\frac{x^2}{4Dt}\right)\right]_0^1 - 50\left[(x-1)\mathrm{erf}\left(\frac{x-1}{\sqrt{4Dt}}\right) + \sqrt{\frac{4Dt}{\pi}}\exp\left(-\frac{(x-1)^2}{4Dt}\right)\right]_0^1$$

$$= \frac{5}{2} + \frac{95}{2}\left[\left(\mathrm{erf}\left(\frac{1}{\sqrt{4Dt}}\right) + \sqrt{\frac{4Dt}{\pi}}\,e^{-\frac{1}{4Dt}} - \sqrt{\frac{4Dt}{\pi}}\right] - 50\left[\sqrt{\frac{4Dt}{\pi}} - \left(-\mathrm{erf}\left(\frac{-1}{\sqrt{4Dt}}\right) + \sqrt{\frac{4Dt}{\pi}}\,e^{-\frac{1}{4Dt}}\right]$$

$$= \frac{5}{2} - \frac{195}{2}\left(\sqrt{\frac{4Dt}{\pi}} - \sqrt{\frac{4Dt}{\pi}}\,e^{-\frac{1}{4Dt}} - \mathrm{erf}\left(\frac{1}{\sqrt{4Dt}}\right)\right)$$

$t=0$ 일 때 $\int_0^1 \rho(x,t)\,dx = 100$.

$\int_0^1 \rho(x,t)\,dx = 50$일 t 값은 $t = 621106\ s \approx 172,5\ h$.

(d). $\int_0^1 \rho(x,t)\,dx = \int_0^1 \left(\frac{5}{2} - \frac{5}{2}\mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right) + 50\,\mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right) - 50\,\mathrm{erf}\left(\frac{x-1}{\sqrt{4Dt}}\right)\right)dx$

위식에서, D와 t는 항상 곱해져 있다.

즉, 동일한 contentration 에 도달하기위한 Dt 값은 일정하며

이때 D가 증가하면 t는 감소. 즉 더 짧은 시간이 소요된다.

2. initial composition of B in A 0.01, surface composition of B 0.05

diffusion coefficient of B in A 4.529×10^{-9} exp $[-147723(J)/RT]$ (m^2/s

temperature range (1173 ~ 1473 k)

(a) 온도가 1173k 일 때 $D = 1.195\times10^{-9}$ cm/s

time	3998s ≈1.1 h	7996s ≈2.2h	11994s ≈3.3h	15992s ≈4.4 h	19990s 5.6h	23988s 6.7h	27986s 7.8h
length	20.1	30.2	36.2	42.2	47.2	51.3	55.3

grid 200 & time 40000s

$\therefore t \propto l^2$

(b) t = 9995s grid 200

temperature(k)	1173 k	1273 k	1373 k	1473 k
Diffusivity (cm^2/s)	1.195×10^{-9}	3.929×10^{-9}	1.086×10^{-8}	2.614×10^{-8}
length (μm)	33.17	60.30	111.56	178.60

$\therefore T \propto \sqrt{l}$

(C) $l \propto \sqrt{t}$ $\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$ 에서 $x \propto \sqrt{Dt}$

$l = a\sqrt{Dt}$ $D = D_0 \exp\left(-\frac{Q}{RT}\right)$ (Q가 activation energy

t = 9995s T=1173k l = 33.17 (μm) $33.17\times10^{-6} = a\sqrt{D_0 \exp\left(-\frac{Q}{8.314\times1173}\right)\times 9995}$

t = 9995s T=1273k l = 60.30 (μm) $60.30\times10^{-6} = a\sqrt{D_0 \exp\left(-\frac{Q}{8.314\times1273}\right)\times 9995}$

$\frac{33.17}{60.30} = \sqrt{\exp\left(-\frac{Q}{8.314\times1173} + \frac{Q}{8.314\times1273}\right)}$ $\boxed{\therefore Q = 148401 \text{ J}}$