HW#7 20212568 강승연

1. Ag-38at% Au alloy (510K)

$C(x,0) = (38\text{at\% Au}) + (12\text{at\% Au})\cos\beta x$

$\uparrow$ wave # $\beta = \frac{2\pi}{\lambda}$ & $\lambda = 2\times10^{-9}\,m$

solution $C(x,t) = (38\text{at\%Au}) + (12\text{at\% Au})\exp[R(\beta)t]\cos\beta x$

$\hookrightarrow \cos\beta x = 1 \rightarrow C_{max} = (38\text{at\% Au}) + (12\text{at\% Au})\exp[R(\beta)t]$

$\cos\beta x = -1 \rightarrow C_{min} = (38\text{at\% Au}) - (12\text{at\% Au})\exp[R(\beta)t]$

$\Rightarrow C_{max} - C_{min} = 2\cdot(12\text{at\% Au})\exp[R(\beta)t]$

Estimate the time / max. composition difference 2at% Au

(a) $\frac{\partial c}{\partial t} = \tilde{D}\frac{\partial^2 c}{\partial x^2}$ $\begin{cases} \frac{\partial c}{\partial t} = R(\beta)(12\text{at\% Au})\exp[R(\beta)t]\cos\beta x \\ \frac{\partial^2 c}{\partial x^2} = -\beta^2(12\text{at\% Au})\exp[R(\beta)t]\cos\beta x \end{cases}$

$\Rightarrow \therefore R(\beta) = -\tilde{D}\beta^2$

$\Rightarrow C_{max} - C_{min} = (24\text{at\% Au})\exp[\underline{R(\beta)}t]$

$= (24\text{at\% Au})\exp[-\tilde{D}\beta^2 t] = 2\%$

$\uparrow$

$\tilde{D} = 10^{-23}\,m^2 s^{-1}$

$\beta = \frac{2\pi}{\lambda} = \frac{2\pi}{2\times10^{-9}m} = \pi\cdot10^{9}m^{-1}$

$\boxed{\therefore t = 251\text{nn sec.}}$

(b) $\underbrace{\frac{\partial c}{\partial t} = \tilde{D}\frac{\partial^2 c}{\partial x^2} - \frac{2K\tilde{D}}{f''}\frac{\partial^4 c}{\partial x^4}}$ $\begin{cases} \frac{\partial c}{\partial t} = R(\beta)(12\text{at\% Au})\exp[R(\beta)t]\cos\beta x \\ \frac{\partial^2 c}{\partial x^2} = -\beta^2(12\text{at\% Au})\exp[R(\beta)t]\cos\beta x \\ \frac{\partial^4 c}{\partial x^4} = \beta^4(12\text{at\% Au})\exp[R(\beta)t]\cos\beta x \end{cases}$

$\Rightarrow \tilde{D}\left[-\beta^2(12\text{at\%})\exp[R(\beta)t]\cos\beta x\right] - \frac{2K\tilde{D}}{f''}\left[\beta^4(12\text{at\%})\exp[R(\beta)t]\cos\beta x\right]$

$\Rightarrow -\exp[R(\beta)t]\cdot\cos\beta x\cdot\tilde{D}\cdot\beta^2\cdot(12\text{at\%})\left[1 + \frac{2K\beta^2}{f''}\right]$

$\therefore \frac{\partial c}{\partial t} = \tilde{D}\frac{\partial^2 c}{\partial x^2} - \frac{2K\tilde{D}}{f''}\frac{\partial^4 c}{\partial x^4} \Rightarrow \therefore R(\beta) = -\tilde{D}\beta^2(1 + 2\frac{K\beta^2}{f''})$

$$C_{max} - C_{min} = (24at\%)\exp[-\tilde{D}\beta^2\cdot(1+2\frac{K\beta^2}{f''})t] = 2\%$$

$$\boxed{\therefore t = 2805n\ sec}$$

$$\begin{cases} \tilde{D} = 10^{-23}\ m^2 \cdot s^{-1} \\ \beta = \frac{2\pi}{\lambda} = \frac{2\pi}{2\times10^{-9}m} = \pi\cdot10^9 m^{-1} \\ f'' = 5\times10^9\ J/m^3 \\ K = -2.6\times10^{-11}\ J/m \end{cases}$$

(c) Au-Ag alloy → $\Delta H_{mix} = X_{Au}X_{Ag}\Omega < 0$

Spinodal decomposition is unfavorable

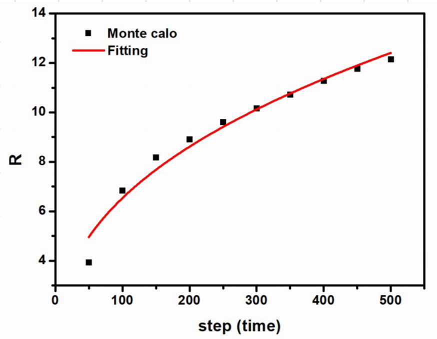
& $\frac{2K\tilde{D}}{f''}\frac{\partial^4 c}{\partial x^4}$; fluctuation term.

(a) & (b) are similar b/c fluctuation term doesn't have a significant impact to time. (this case is not spinodal decomposition)

∴ answer (a) & (b) is not large different.

$\boxed{2}$ (a) $R = Kt^n$

Step : 500
(500step의 sample을 T=5, 10, 15, 20에서 각각 solve)



- step : 500 (per 50 step)
- temperature : 20

fitting eqn. $y = ax^b$

$\Rightarrow \begin{cases} a = 1.04 \\ b = 0.39 \simeq 0.4 \end{cases}$

(b)

$$R = Kt^n = K_0\exp(-\frac{Q}{kT})\cdot t^n$$

$$\ln R = \ln K_0 t^n - \frac{Q}{k}\cdot\frac{1}{T} \leftarrow \text{fitting eqn ; } y = ax + b$$

$$a = -\frac{Q}{k} = -0.4926$$