HW7 화학과 손예림

1.

(a)

$$\frac{\partial C}{\partial t} = \tilde{D}\frac{\partial^2 C}{\partial x^2}$$

$$\frac{\partial C}{\partial t} = R(\beta)(12\ \text{at\%}\ Au)\exp[R(\beta)t]\cos\beta x$$

$$\frac{\partial^2 C}{\partial x^2} = -\beta^2(12\ \text{at\%}\ Au)\exp[R(\beta)t]\cos\beta x$$

$$\Rightarrow R(\beta)(12\ \text{at\%}\ Au)\exp[R(\beta)t]\cos\beta x = -\tilde{D}\beta^2(12\ \text{at\%}\ Au)\exp[R(\beta)t]\cos\beta x$$

$$\Rightarrow R(\beta) = -\tilde{D}\beta^2 \quad \cdots ①$$

$C_{max} = (38\ \text{at\%}\ Au) + (12\ \text{at\%}\ Au)\exp[R(\beta)t]$ at $\beta x = n\pi$ & n is even number

$C_{min} = (38\ \text{at\%}\ Au) - (12\ \text{at\%}\ Au)\exp[R(\beta)t]$ at $\beta x = n\pi$ & n is odd number

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

$$\Rightarrow 12\exp[R(\beta)t] = 1 \quad \cdots ②$$

①을 ②에 대입

$$12\exp[-\tilde{D}\beta^2 t] = 1$$

$$\Rightarrow t = \frac{\ln(12)}{\tilde{D}\beta^2} = \frac{\ln(12)}{(10^{-23}\ m^2 s^{-1})\left(\frac{\pi}{10^{-9}\ m}\right)^2} \simeq 25177\ s$$

$\therefore t \simeq 25177\ s$

(b)

$$\frac{\partial C}{\partial t} = \tilde{D}\frac{\partial^2 C}{\partial x^2} - \frac{2K\tilde{D}}{f''}\frac{\partial^4 C}{\partial x^4}$$

$$\frac{\partial^4 C}{\partial x^4} = \beta^4(12\ \text{at\%}\ Au)\exp[R(\beta)t]\cos\beta x$$

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

$$\Rightarrow R(\beta) = -\tilde{D}\beta^2 - \frac{2KD}{f''}\beta^4 \quad \cdots ③$$

③을 (a)의 ②에 대입하여 정리

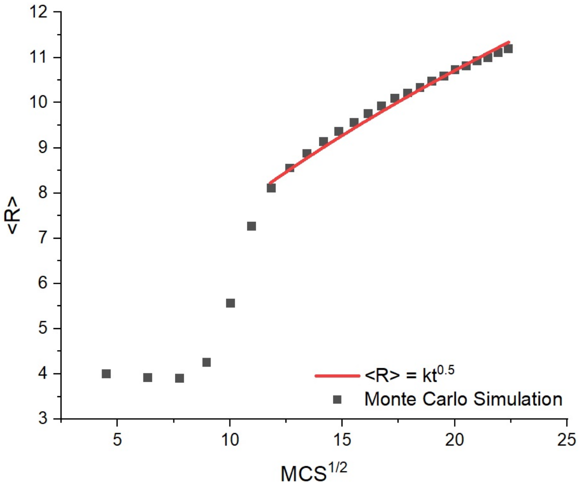
$$\Rightarrow t = \frac{\ln(12)}{\tilde{D}\beta^2 + \frac{2KD}{f''}\beta^4} = \frac{\ln(12)}{(10^{-23}\,m^2 s^{-1})\left(\frac{\pi}{10^{-9}\,m}\right)^2 + \frac{2(-2.6\times10^{-11}\,J\,m^{-1})(10^{-23}\,m^2 s^{-1})}{(5\times10^9\,J\,m^{-3})}\left(\frac{\pi}{10^{-9}\,m}\right)^4}$$

$$\simeq 28057\,s$$

$$\therefore t = 28057\,s$$

(c)
계면에너지를 고려할 경우 Ag-Au system은 spinodal decomposition을 덜 선호한다.
Ag-Au system은 원자와 달리 결합을 선호하고 negative gradient energy coefficient를 가지기 때문에 spinodal decomposition을 덜 선호하는 (b)의 답이 더 적절하다.

2.
(a)



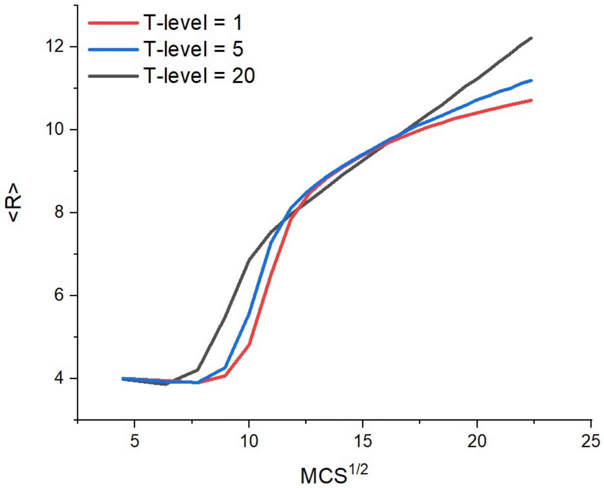
for ideal grain growth, $R^2 - R_0^2 = kt$

(R : final grain size, R_0 : initial grain size)

$\Rightarrow \langle R \rangle = k t^{1/2}$

for T-level = 5, $k \simeq 2.395$

(b)



for T-level = 1, $k \simeq 2.363$

for T-level = 5, $k \simeq 2.395$

for T-level = 20, $k \simeq 2.458$

$$\langle R \rangle = k t^n = k_0 e^{-\frac{Q}{RT}} t^n$$

$$\Rightarrow \ln k = \ln k_0 - \frac{Q}{RT}$$

연립방정식을 이용하면

$k_0 \simeq 2.449$

$\frac{Q}{R} \simeq 0.07714$