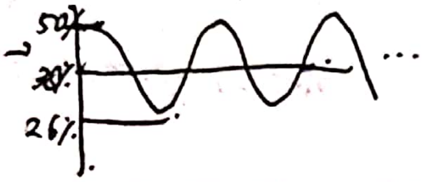
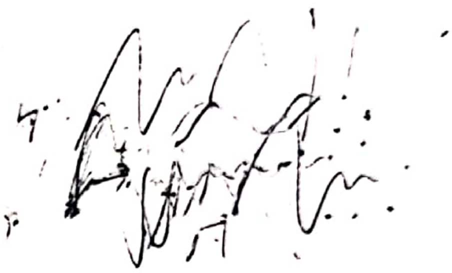
상변태론 HW7 20170330 이윤호

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

초기 composition profile →





시간 t에서의 composition : $C(x,t) = 38\,at\% + 12\,at\%\cdot\exp[R(\beta)t]\cos\beta x.$

(a). Fick's law를 사용하여 diffusion equation을 풀면,

$$\frac{\partial C}{\partial t} = 12R(\beta)\exp[R(\beta)t]\cos\beta x.$$

$$\tilde{D}\frac{\partial^2 C}{\partial x^2} = -12\beta^2\tilde{D}\exp[R(\beta)t]\cos\beta x.$$

$$\therefore\ 12R(\beta)\exp[R(\beta)t]\cos\beta x = -12\beta^2\tilde{D}\exp[R(\beta)t]\cos\beta x.$$

$$\therefore\ R(\beta) = -\tilde{D}\beta^2 = -10^{-23}\,m^2/s\left(\frac{2\pi}{(2\times10^{-9})m}\right)^2 = -9.9\times10^{-5}/s$$

$$C(x,t) = 38 + 12\exp(-9.9\times10^{-5}t)\cos\beta x.$$

maximum composition difference가 2가 되려면.

$$C(0,t) = 39 = 38 + 12\exp(-9.9\times10^{-5}t) \Rightarrow t = 25200\,s.$$

(b) Fick's law가 아니라 modified diffusion equation을 쓴다면,

$$\frac{\partial C}{\partial t} = 12R(\beta)\exp[R(\beta)t]\cos\beta x.$$

$$\tilde{D}\frac{\partial^2 C}{\partial x^2} - \frac{2K\tilde{D}}{f''}\frac{\partial^4 C}{\partial x^4} = \left(-\tilde{D}\beta^2 - \frac{2K\tilde{D}}{f''}\beta^4\right)\cdot 12\exp[R(\beta)t]\cos\beta x$$

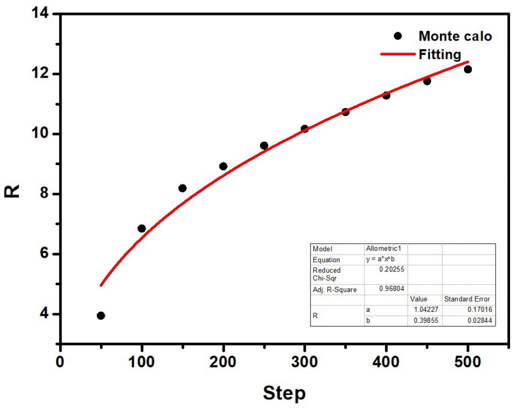
$$\therefore\ R(\beta) = -\tilde{D}\beta^2 - \frac{2K\tilde{D}}{f''}\beta^2 = -1.08\times10^{-4}/s.$$

$$C(0,t) = 38 + 12\exp(-1.08\times10^{-4}t) = 39. \Rightarrow t = 23008\,s.$$

(c) Ag와 Au가 ordering phase를 이룬다는 것은. Ag와 Au가 서로 잘 결합한다는 것이다. ($\varepsilon_{Ag-Au} > \frac{1}{2}(\varepsilon_{Ag-Ag} + \varepsilon_{Au-Au})$) ΔH_{mix}이 음수가 되게되고, 이경우. ΔG_{mix}는 항상 음수가 되어 miscibility gap이 나타날수 없다 ⇔ $\frac{d^2G}{dX^2} > 0$.

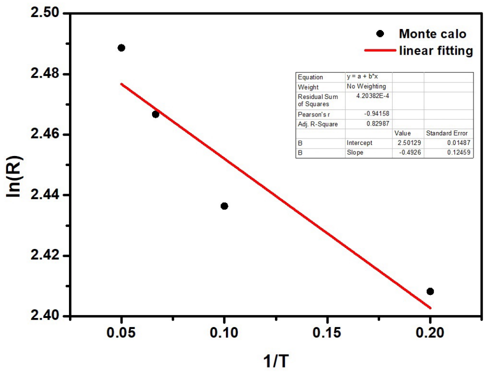
spinodal decomposition은 miscibility gap 내에서, 즉 $\frac{d^2G}{dX^2} < 0$ 인구간에서만 나타나므로 Ag-Au system에서는 일어나지 않는것이다.

spinodal decomposition이 일어나지 않으면 uphill diffusion이 일어나지 않고 ($\tilde{D}$가 양수인 것으로 확인가능) Au는 concentration gradient에 의해 확산되기 때문에 Fick's law나 Cahn equation이나 큰 의미차이는 없은것이다.



(a) $R = kt^n$. simulation 결과. $y = ax^b \rightarrow a = 1.042$

$b = 0.399$



(b) $R = kt^n = K_0 \exp\left(\frac{-Q}{kT}\right) t^n$.

($\because$ boundary migration is thermally activated process)

$\Rightarrow \ln R = \ln K_0 t^n - \frac{Q}{K} \cdot \frac{1}{T}$ (time is constant)

simulation 결과 $y = a + bx$ $\quad b = -0.493$

$= -\frac{Q}{K}$

$Q = 0.493k$ (k: Boltzmann constant)