HW 4 화학과 손예림

1.

nucleation이 발생하기 위한 energy barrier, ΔG^*는 다음을 통해 구할 수 있다.

$$\Delta G = \frac{4}{3}\pi r^3 \Delta G_v + 4\pi r^2 \gamma \qquad (\text{when } \Delta G_v < 0)$$

$$\left.\frac{\partial \Delta G}{\partial r}\right|_{r=r^*} = 4\pi r^{*2} \Delta G_v + 8\pi r^* \gamma = 0.$$

$$r^* = -\frac{2\gamma}{\Delta G_v}, \quad \Delta G^* = \frac{16\pi \gamma^3}{3(\Delta G_v)^2}$$

homogeneous nucleation 이 일어나며, 구형의 핵이 형성될 때 nucleation rate, I는 다음과 같다.

$$I = f_0 N_0 \exp\left(-\frac{\Delta G^*}{kT}\right)$$

$$\Rightarrow \ln I = \ln f_0 N_0 - \frac{\Delta G^*}{kT}$$

즉, $\ln I$ vs $1/T$ 그래프의 기울기는 $-\frac{\Delta G^*}{k}$와 같다.

$$-23.8 \times 10^3 \ K = -\frac{\Delta G^*}{k} = -\frac{1}{k}\frac{16\pi\gamma^3}{3(\Delta G_v)^2}$$

$$\Rightarrow \gamma = \sqrt[3]{(23.8\times10^3 \ K)\times k \times \frac{3(\Delta G_v)^2}{16\pi}}$$

$$= \sqrt[3]{(23.8\times10^3 \ K)\times(1.38\times10^{-23} \ J/K)\times\frac{3(-10^8 \ J/m^3)^2}{16\pi}}$$

$$= 0.058 \ J/m^2$$

∴ liquid-solid interfacial energy for tin = $0.058 \ J/m^2$

(b)

(a)에서 구한 바와 같이

$$r^* = -\frac{2\gamma}{\Delta G_v} = -\frac{2\times(0.058 \ J/m^2)}{-10^8 \ J/m^3} = 1.16\times10^{-9} m = 1.16 \ nm$$

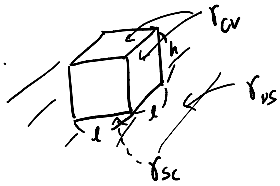
(c)

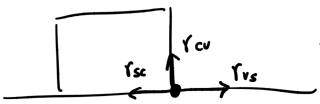
# of tin atoms in a nucleus of critical size = $\frac{\text{volume of nucleus of critical size}}{\text{volume of tin atom}}$

$$= \frac{\frac{4}{3}\pi\times(1.16\times10^{-9} m)^3}{\frac{4}{3}\pi\times(1.5\times10^{-10} m)^3} = 462.48$$

∴ 462 개

2.





$\Rightarrow \gamma_{sc} = \gamma_{vs}$

$$\Delta G = -V_{solid}\,\Delta G_v + \sum_j A_j \gamma_j$$

$$= -l^2 h\,\Delta G_v + l^2\gamma_{sc} + 4lh\gamma_{cv} + l^2\gamma_{cv} - l^2\gamma_{vs}$$

$$= -l^2 h\,\Delta G_v + (4lh + l^2)\gamma_{cv} \qquad (\because \gamma_{sc} = \gamma_{vs})$$

ΔG를 l, h로 각각 편미분하여 0이 되는 critical size, l^*와 h^*를 구하자.

$$\left.\frac{\partial \Delta G}{\partial h}\right|_{h=h^*,\,l=l^*} = -l^{*2}\Delta G_v + 4l^*\gamma_{cv} = 0$$

$$\Rightarrow l^* = \frac{4\gamma_{cv}}{\Delta G_v}$$

$$\left.\frac{\partial \Delta G}{\partial l}\right|_{h=h^*,\,l=l^*} = -2l^* h^*\Delta G_v + (4h^* + 2l^*)\gamma_{cv}$$

$$= -8\gamma_{cv}h^* + 4h^*\gamma_{cv} + \frac{8\gamma_{cv}^2}{\Delta G_v}$$

$$= -4\gamma_{cv}\left(h^* - \frac{2\gamma_{cv}}{\Delta G_v}\right) = 0$$

$$\Rightarrow h^* = \frac{2\gamma_{cv}}{\Delta G_v}$$

$$\Delta G^* = -\left(\frac{4\gamma_{cv}}{\Delta G_v}\right)^2\left(\frac{2\gamma_{cv}}{\Delta G_v}\right)\Delta G_v + \left[4\left(\frac{4\gamma_{cv}}{\Delta G}\right)\left(\frac{2\gamma_{cv}}{\Delta G_v}\right) + \left(\frac{4\gamma_{cv}}{\Delta G}\right)^2\right]\gamma_{cv}$$

$$= \frac{16\gamma_{cv}^3}{\Delta G_v^2}$$

$$\therefore\ l^* = \frac{4\gamma_{cv}}{\Delta G_v}, \quad h^* = \frac{2\gamma_{cv}}{\Delta G_v}, \quad \Delta G^* = \frac{16\gamma_{cv}^3}{\Delta G_v^2}$$