

HW4 20190330 야정준

1. (a) homogeneous nucleation, nucleus \rightarrow spherical.
total Gibbs free energy change in system $\Rightarrow \Delta G$

$$\Delta G = +\frac{4}{3}\pi r^3 \Delta G_V + 4\pi r^2 \gamma \quad (\Delta G_V < 0)$$

at critical radius $r^* \rightarrow \frac{d\Delta G}{dr} \Big|_{r=r^*} = 0$

$$\frac{d\Delta G}{dr} = +4\pi r^2 \Delta G_V + 8\pi r \gamma = 0 \quad r = r^* = -\frac{2\gamma}{\Delta G_V}$$

energy barrier for nucleation (ΔG^*) = $\frac{16\pi\gamma^3}{3(\Delta G_V)^2}$

Homogeneous nucleation rate (I) is proportionally increase with the number of nuclei size with r^* .

$\Rightarrow I = f_0 G_0 \exp\left(-\frac{\Delta G^*}{kT}\right)$ Boltzmann distribution.

$$\ln I \propto -\frac{\Delta G^*}{kT} \quad \ln I \propto -\frac{\Delta G^*}{k} = -\frac{16\pi\gamma^3}{3k(\Delta G_V)^2} = -23.8 \times 10^3$$

$\gamma = 0.27 \text{ J/m}^2$

(b) $r^* = \frac{2\gamma}{-\Delta G_V} = -\frac{2 \times 0.27 \text{ J/m}^2}{-10^8 \text{ J/m}^3} = 5.4 \times 10^{-9} \text{ m}$

(c) $V_{\text{nuclei}} = \frac{4}{3}\pi r^{*3} \quad V_{\text{in atom}} = \frac{4}{3}\pi r_{\text{atom}}^3$

$$\frac{V_{\text{nuclei}}}{V_{\text{atom}}} = \frac{(5.4 \times 10^{-9})^3}{(1.5 \times 10^{-10})^3} = 46656 \text{ atoms/nuclei}$$

2. (cubic particles) \Rightarrow System total Gibbs free E $\Delta G =$

$$\Delta G = -V\Delta G_V + \Delta A \gamma_c$$

$$\Rightarrow \Delta G = -l^3 \Delta G_V + l^2 (\gamma_{sc} + \gamma_{cv} - \gamma_{sv}) + 4l^2 h \gamma_{cv}$$

Assume constant volume. $V = l^2 h \rightarrow \frac{dh}{dl} = -\frac{2h}{l}$

$$\frac{\partial \Delta G}{\partial l} = -2lh\Delta G_V - l^2 \frac{dh}{dl} \Delta G_V + 2l(\gamma_{sc} + \gamma_{cv} - \gamma_{sv}) + 4h\gamma_{cv} + 4l \frac{dh}{dl} \gamma_{cv} = 0 \quad (l = l^*)$$

$$0 = -\Delta G_V + 2l(\gamma_{sc} + \gamma_{cv} - \gamma_{sv}) - 4h\gamma_{cv}$$

$$\left(\frac{l^*}{h}\right) = \frac{2\gamma_{cv}}{\gamma_{sc} + \gamma_{cv} - \gamma_{sv}}$$

$$l = \frac{2\gamma_{cv}}{\gamma_{sc} + \gamma_{cv} - \gamma_{sv}} = \frac{2\gamma_{cv} h}{A}$$

$$\Delta G = -\Delta G_V \cdot \frac{A}{2\gamma_{cv}} l^3 + A l^2 + 2A l^2 = -\Delta G_V \cdot \frac{A}{2\gamma_{cv}} l^3 + 3A l^2$$

$$\frac{d\Delta G}{dl} = -\frac{3A\Delta G_V}{2\gamma_{cv}} l^2 + 6Al = 0 \quad l^2 = \frac{4\gamma_{cv}}{\Delta G_V}$$

$$h^* = \frac{Al}{2\gamma_{cv}} = \frac{2(\gamma_{sc} + \gamma_{cv} - \gamma_{sv})}{\Delta G_V}$$

$$\Delta G^* = \frac{16\gamma_{cv}^2}{\Delta G_V^2} (\gamma_{sc} + \gamma_{cv} - \gamma_{sv})$$