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1. nucleation vapor → liquid

$$dG = -SdT + VdP + \sum_i \mu_i dn_i + \gamma dA$$

↓ T, P const.

$$dG = \mu_{vap} dn_{vap} + \mu_{liq} dn_{liq} + \gamma dA$$

$$= -(\mu_{vap} - \mu_{liq}) dn_{liq} + \gamma dA$$

$+(\mu_{vap} - \mu_{liq}) = \Delta G_{vap}$ (per volume of liquid)

$$\Delta G = -\Delta G_{vap} \cdot \left(\frac{4}{3}\pi r^3\right) + 4\pi r^2 \gamma$$

- V_m : ~~molar volume~~ atomic volume

  n : number of atoms in cluster

  $\frac{4}{3}\pi r^3 = n \cdot V_m$, $r^3 = \frac{3nV_m}{4\pi}$, $r = \left(\frac{3nV_m}{4\pi}\right)^{\frac{1}{3}}$

  $4\pi r^2 = 4\pi \left(\frac{3nV_m}{4\pi}\right)^{\frac{2}{3}} = 4^{\frac{1}{3}} 9^{\frac{1}{3}} \pi^{\frac{1}{3}} \cdot n^{\frac{2}{3}} \cdot V_m^{\frac{2}{3}} = (36\pi)^{\frac{1}{3}} \cdot n^{\frac{2}{3}} \cdot V_m^{\frac{2}{3}}$

$$\therefore \Delta G = -\Delta G_{vap} \cdot (nV_m) + (36\pi)^{\frac{1}{3}} \cdot n^{\frac{2}{3}} \cdot V_m^{\frac{2}{3}} \cdot \gamma$$

2.

(a) $\Delta G_n = -n\nu\Delta G_v + (36\pi)^{\frac{1}{3}} \cdot n^{\frac{2}{3}} \cdot \nu^{\frac{2}{3}} \gamma$

(b) $\frac{d\Delta G}{dn} = 0 \Rightarrow \left.\frac{d\Delta G}{dn}\right|_{n^*} = -\nu\Delta G_v + (36\pi)^{\frac{1}{3}} \cdot \frac{2}{3} n^{*-\frac{1}{3}} \cdot \nu^{\frac{2}{3}} \gamma = 0$

$$\Rightarrow n^* = \left(\frac{(36\pi)^{\frac{1}{3}} \cdot 2 \cdot \nu^{\frac{2}{3}} \cdot \gamma}{3\nu\Delta G_v}\right)^3 = \frac{36\pi}{3} \cdot \frac{2^3}{\nu} \left(\frac{\gamma}{\Delta G_v}\right)^3$$

$$= \frac{32}{3} \frac{\pi}{\nu} \left(\frac{\gamma}{\Delta G_v}\right)^3$$

(c)

$$\Delta G_{dia} = -n(G_{vap} - G_{dia}) + (36\pi)^{\frac{1}{3}} \cdot n^{\frac{2}{3}} \cdot V_{dia}^{\frac{2}{3}} \gamma_{dia}$$

$$\Delta G_{gr} = -n(G_{vap} - G_{gr}) + (36\pi)^{\frac{1}{3}} \cdot n^{\frac{2}{3}} \cdot \nu_{gr}^{\frac{2}{3}} \cdot \gamma_{gr}$$

$$\Delta G_{dia} = \Delta G_{gr}$$

$$n(G_{dia} - G_{gr}) = (36\pi)^{\frac{1}{3}} \cdot n^{\frac{2}{3}} (\nu_{gr}^{\frac{2}{3}} \cdot \gamma_{gr} - \nu_{dia}^{\frac{2}{3}} \gamma_{dia})$$

$$n = \left[\frac{(36\pi)^{\frac{1}{3}} \cdot (\nu_{gr}^{\frac{2}{3}} \cdot \gamma_{gr} - \nu_{dia}^{\frac{2}{3}} \gamma_{dia})}{(G_{dia} - G_{gr})}\right]^3$$

if $\gamma_{dia} = 3.6$

$$n = \left(\frac{(36\pi)^{\frac{1}{3}} \cdot (8\times10^{-30})^{\frac{2}{3}} \times 3.1 - (6\times10^{-30})^{\frac{2}{3}} \times 3.6}{0.02 \times 1.602 \times 10^{-19}}\right)^3 \simeq 464$$

if $\gamma_{dia} = 3.65$, if $\gamma_{dia} = 3.70$

$n \simeq 145$ $\quad$ $n \simeq 21$

d)

$$\Delta G_{dia} < \Delta G_{gr}$$

$$\Rightarrow n < \left[\frac{(36\pi)^{\frac{1}{3}} \cdot (V_{gr}^{\frac{2}{3}} \cdot \gamma_{gr} - V_{dia}^{\frac{2}{3}} \cdot \gamma_{dia})}{(G_{dia} - G_{gr})} \right]^3$$

e)

$$n^* = \frac{32\pi}{3V_{gr}} \left(\frac{\gamma_{gr}}{\Delta G_{v,gr}} \right)^3 \Rightarrow \Delta G_{v,gr} = \left(\frac{32\pi}{3V_{gr} \cdot n^*} \right)^{\frac{1}{3}} \cdot \gamma_{gr}$$

$$= \left(\frac{32\pi}{3 \cdot (8\times10^{-30}) \cdot 100} \right)^{\frac{1}{3}} \cdot 3.1$$

$$= 1.077 \times 10^{10}\ J/m^3$$

f)

$$\frac{I_{gr}}{I_{dia}} = \frac{A \exp\left(\frac{-\Delta G^*_{v,gr}}{kT}\right)}{A \exp\left(\frac{-\Delta G^*_{v,dia}}{kT}\right)} = \exp\left(-\frac{\Delta G^*_{v,gr}}{kT} + \frac{\Delta G^*_{v,dia}}{kT} \right)$$

$$= \exp\left(\frac{-\frac{16}{3}\pi \frac{\gamma_{gr}^3}{\Delta G_{v,gr}^2} + \frac{16}{3}\pi \frac{\gamma_{dia}^3}{\Delta G_{v,dia}^2}}{kT} \right)$$

$$= \exp\left(\frac{16}{3}\frac{\pi}{kT} \left(-\frac{\gamma_{gr}^3}{\Delta G_{v,gr}^2} + \frac{\gamma_{dia}^3}{\Delta G_{v,dia}^2} \right) \right)$$

- $\Delta G_{v,gr} = 1.077 \times 10^{10} J/m^3$
- $G^\circ_{dia} - G^\circ_{gr} = V_{gr} \cdot \Delta G_{v,gr} - V_{dia} \cdot \Delta G_{v,dia}$

$$\Delta G_{v,dia} = \frac{V_{gr} \cdot \Delta G_{v,gr} - (G^\circ_{dia} - G^\circ_{gr})}{V_{dia}} = \frac{(8\times10^{-30}) \cdot (1.077\times10^{10}) - (0.02 \times 1.6077\times10^{-19})}{6\times10^{-30}}$$

$$= 1.38 \times 10^{10}\ J/m^3$$

- If $T = 298K$, $\gamma_{dia} = 3.6$

$$\frac{I_{gr}}{I_{dia}} = \exp\left(\frac{16\pi}{3 \cdot 1.38\times10^{-23} \times 298} \left(-\frac{3.1^3}{(1.077\times10^{10})^2} + \frac{3.6^3}{(1.38\times10^{10})^2} \right) \right)$$

$$= 1.103 \times 10^{-21}$$

If $T = 298K$, $\gamma_{dia} = 3.65$

$$\frac{I_{gr}}{I_{dia}} = 2.274 \times 10^{-3}$$

If $T = 298K$, $\gamma_{dia} = 3.7$

$$\frac{I_{gr}}{I_{dia}} = 1.514 \times 10^{16}$$

g) bulk 상태에서는 graphite 가 diamond 보다 안정하지만 nano size에서는 surface에 의한 영향을 많이 받아 diamond 가 더 잘 형성될 수 있다.

γ_{dia} 가 ~~[illegible]~~ 작을 수록 diamond가 더 잘 형성 된다.

h) $CH_4 \rightarrow C + H_2$ 반응이 일어나면 C의 분압이 증가한다. 이 때 graphite가 형성된다는 것은 critical number of atom of graphite를 줄였다는 것이다.

이를 줄이기 위해서는 $\Delta G_{v,gr}$, driving force가 증가했음을 알 수 있다.

즉, driving force of graphite는 C 분압과 연관 있음을 알 수 있다.

CamScanner로 스캔하기