상변태론 HW#5 20222660 이송

1. (a) $\Delta G = -\frac{4}{3}\pi r^3 \Delta G_v + 4\pi r^2 \gamma$

$\frac{4}{3}\pi r^3 = n \cdot V \Rightarrow r = \left(\frac{3}{4\pi}\right)^{1/3} n^{1/3} \cdot V^{1/3}$

$\Delta G = -nV\Delta G_v + 4\pi\gamma \cdot \left(\frac{9}{16\pi^2}\right)^{1/3} \cdot n^{2/3} \cdot V^{2/3}$

$= -n\Delta G_a + \left(\frac{64\pi^3 \times 9}{16\pi^2}\right)^{1/3} \cdot n^{2/3} \cdot V^{2/3} \cdot \gamma$

$= \boxed{-n\Delta G_a + (36\pi)^{1/3} \cdot n^{2/3} \cdot V^{2/3} \cdot \gamma}$

(b) for $n = n^*$, $\frac{\partial \Delta G}{\partial n} = 0$.

$\left.\frac{\partial \Delta G}{\partial n}\right|_{n=n^*} = -V\Delta G_v + (36\pi)^{1/3} \cdot V^{2/3} \cdot \gamma \cdot \frac{2}{3} n^{*-\frac{1}{3}} = 0 \Leftrightarrow n^{*\frac{1}{3}} = \frac{\gamma}{\Delta G_v} \cdot (36\pi)^{1/3} \cdot V^{-1/3} \cdot \frac{2}{3}$

$n^* = \left(\frac{\gamma}{\Delta G_v}\right)^3 \cdot 36\pi \cdot V^{-1} \cdot \frac{8}{27}$

$n^* = \boxed{\left(\frac{\gamma}{\Delta G_v}\right)^3 \cdot \frac{32\pi}{3V}}$

$\Delta G^* = -n^* V\Delta G_v + (36\pi)^{1/3} \cdot n^{*2/3} \cdot V^{2/3} \cdot \gamma$

$= -\frac{32\pi}{3} \cdot \frac{\gamma^3}{\Delta G_v^2} + (36\pi)^{1/3} \cdot \frac{\gamma^2}{\Delta G_v^2} \cdot \left(\frac{32\pi}{3}\right)^{2/3} \cdot \gamma$

$= \frac{\gamma^3}{\Delta G_v^2}\left[-\frac{32\pi}{3} + \left(6\pi^{1/2} \cdot \frac{32\pi}{3}\right)^{2/3}\right] = \boxed{\frac{16\pi}{3}\frac{\gamma^3}{\Delta G_v^2}}$

(c) stability 가 같음 $\Rightarrow \Delta G_{dia} = \Delta G_{gra} \rightarrow -n\Delta G_{a,dia} + (36\pi)^{1/3} \cdot n^{2/3} \cdot V_{dia}^{2/3} \cdot \gamma_{dia}$

$= -n\Delta G_{a,gra} + (36\pi)^{1/3} \cdot n^{2/3} \cdot V_{gra}^{2/3} \cdot \gamma_{gr}$

$n = 36\pi\left(\frac{V_{gr}^{2/3}\gamma_{gr} - V_{dia}^{2/3}\gamma_{dia}}{G^\circ_{dia} - G^\circ_{gr}}\right)^3$ ← n로 정리.

세가지 조건 대입.

i) $\gamma_{dia} = 3.6 Jm^{-2}$

$n = 36\pi\left(\frac{(8\times10^{-30})^{2/3} \cdot 3.1 - (6\times10^{-30})^{2/3} \cdot 3.6}{0.02 \times 1.6 \times 10^{-19}}\right)^3 = 466.14$ $\boxed{\therefore 466 \text{atoms}}$

ii) $\gamma_{dia} = 3.65 Jm^{-2}$ $\boxed{\therefore 145 \text{atoms}}$

iii) $\gamma_{dia} = 3.7 Jm^{-2}$ $\boxed{\therefore 21 \text{atoms}}$

(d) size와 상관없이 diamond가 안정하려면

$\Delta G_{dia} < \Delta G_{gra}$.

등식 대신 부등식으로 똑같이 풀면, $n < 36\pi\left(\frac{V_{gr}^{2/3}\gamma_{gr} - V_{dia}^{2/3}\gamma_{dia}}{G^\circ_{dia} - G^\circ_{gr}}\right)^3$

(e) $n^* = \left(\frac{\gamma}{\Delta G_v}\right)^3 \cdot \frac{32\pi}{3V} = 100$

$\Delta G_v = \left[(3.1)^3 \cdot \frac{32\pi}{3} \cdot \frac{1}{8\times10^{-30}} \cdot \frac{1}{100}\right]^{1/3} = 10.76\times10^{9}\ \mathrm{J\,m^{-3}}$

(f) $\frac{I_{gra}}{I_{dia}} = \frac{A\cdot\exp(-\Delta G^*_{gra}/kT)}{A\cdot\exp(-\Delta G^*_{dia}/kT)} = \exp\left(\frac{\Delta G^*_{dia} - \Delta G^*_{gra}}{kT}\right) =$

ΔG^*_{gra}는 여기서 $\frac{16\pi}{3}\frac{\gamma^3}{\Delta G_{V,gra}}$ 으로 계산. 4.28×10^{-18}

ΔG^*_{dia} 구하려면 $\Delta G_{V,dia}$가 필요.

$G^\circ_{dia} - G^\circ_{gr} = 0.02\ \mathrm{eV/atom}$

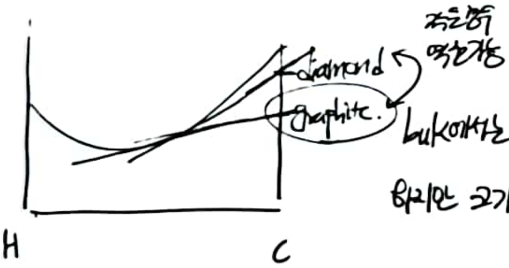
$= V_{dia}\Delta G_{V,dia} - V_{gra}\Delta G_{gra}$. 이용으로 구하기.

$\therefore \Delta G_{V,dia} = 1.39\times10^{10}\ \mathrm{Jm^{-2}}$

$\therefore \frac{I_{gra}}{I_{dia}} = \exp\left(\frac{\frac{16\pi}{3}\cdot\frac{\gamma_{dia}^3}{(1.39\times10^{10})^2} - 4.28\times10^{-18}}{0.026\times1.6\times10^{-19}}\right) = 6.7\times10^{-26},\ 5.1\times10^{7},\ 3.5\times10^{11}$

$\gamma_{dia} = 3.6\ \mathrm{Jm^{-2}}$, $3.65\ \mathrm{Jm^{-2}}$, $3.7\ \mathrm{Jm^{-2}}$

(g)



bulk에서는 graphite가 더안정하기 때문에 생성 잘안됨.

하지만 크기가 작아지면 diamond가 더 stable 해질 수 있음

이 stable 해지는 정도는 γ_{dia} 에 의해 조금만 바뀌어도 크게 변화됨.

$\therefore$ γ_{dia}가 작아질 수 있는 작은 효과만 있더라도 diamond 생성 ⇑

CVD의 경우에는 표면 charge.