20212145 채민지.

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

구의부피 = 원자 개수 × 원자하나 부피

$\frac{4}{3}\pi r^3 = n\nu \rightarrow r = \left(\frac{3n\nu}{4\pi}\right)^{1/3}$

$4\pi r^2 = (36\pi)^{\frac{1}{3}} n^{2/3} \nu^{2/3}$

$\Rightarrow \Delta G = -n\nu\Delta G_V + (36\pi)^{1/3} n^{2/3} \nu^{2/3} \gamma$

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

$(36\pi)^{1/3} \frac{2}{3} n^{*-1/3} \nu^{2/3} \gamma = \nu \Delta G_V$

$n^{*\frac{1}{3}} = (36\pi)^{1/3} \left(\frac{8}{3}\right)^{\frac{1}{3}} \frac{\gamma}{\nu^{1/3} \Delta G_V}$

$n^* = \frac{32\pi\gamma^3}{3\nu\Delta G_V^3} \Rightarrow \Delta G^* = -\frac{32\pi\gamma^3}{3\nu\Delta G_V^3}\nu\Delta G_V + (36\pi)^{1/3}\left(\frac{32\pi}{3}\right)^{2/3} \frac{\gamma^2}{\Delta G_V^2} \left(\frac{1}{\nu}\right)^{2/3} \nu^{2/3}\gamma$

$= \frac{16\pi}{3}\frac{\gamma^3}{\Delta G_V^2}$

(c) $\Delta G_{gr} = -n(^\circ G_V - {}^\circ G_{gr}) + (36\pi)^{1/3} n^{2/3} \nu_{gr}^{2/3} \gamma_{gr}$

$\Delta G_{dia} = -n(^\circ G_V - {}^\circ G_{dia}) + (36\pi)^{1/3} n^{2/3} \nu_{dia}^{2/3} \gamma_{dia}$

$\Delta G_{gr} = \Delta G_{dia} \Rightarrow -n(^\circ G_V - {}^\circ G_{gr}) + (36\pi)^{1/3} n^{2/3} \nu_{gr}^{2/3} \gamma_{gr} = -n(^\circ G_V - {}^\circ G_{dia}) + (36\pi)^{1/3} n^{2/3} \nu_{dia}^{2/3} \gamma_{dia}$

$\Rightarrow \quad n(^\circ G_{gr} - {}^\circ G_{dia}) = n^{2/3}(36\pi)^{1/3}(\nu_{dia}^{2/3}\gamma_{dia} - \nu_{gr}^{2/3}\gamma_{gr})$

$n = 36\pi \left(\frac{\nu_{dia}^{2/3}\gamma_{dia} - \nu_{gr}^{2/3}\gamma_{gr}}{^\circ G_{gr} - {}^\circ G_{dia}}\right)^3$

1) $\gamma_{dia} = 3.6 J/m^2$ $\quad n = 36\pi \left(\frac{(6\times10^{-30} m^3/atom)^{2/3}(3.6 \times \frac{1}{1.6\times10^{-19}} eV/m^2) - (8\times10^{-30} m^3/atom)^{2/3}(3.1 \times \frac{1}{1.6\times10^{-19}} eV/m^2)}{-0.02 eV/atom}\right)^3$

$(1eV = 1.6 \times 10^{-19} J) \quad \simeq 465$ (개)

2) $\gamma_{dia} = 3.65 J/m^2$ $\quad n = 36\pi \left(\frac{(6\times10^{-30})^{2/3}(3.65 \times \frac{1}{1.6\times10^{-19}}) - (8\times10^{-30})^{2/3}(3.1 \times \frac{1}{1.6\times10^{-19}})}{-0.02}\right)^3$

$\simeq 146$ (개)

3) $\gamma_{dia} = 3.70 J/m^2$ $\quad n = 36\pi \left(\frac{(6\times10^{-30})^{2/3}(3.7 \times \frac{1}{1.6\times10^{-19}}) - (8\times10^{-30})^{2/3}(3.1 \times \frac{1}{1.6\times10^{-19}})}{-0.02}\right)^3$

$\simeq 210$ (개)

(d) diamond cluster가 graphite 보다 안정하려면,

$\Delta G_{dia} < \Delta G_{gr}$ 을 만족 하면 된다. (모든 size 에서)

$\Delta G_{dia} - \Delta G_{gr} < 0$

$\therefore n < 36\pi \left(\frac{V_{dia}^{2/3}\gamma_{dia} - V_{gr}^{2/3}\gamma_{gr}}{{}^{\circ}G_{gr} - {}^{\circ}G_{dia}} \right)^3$ 식을 만족해야 한다

(e)

$$n^* = 100 = \frac{32\pi\gamma_{gr}^3}{3V_{gr}\Delta G_{V_{gr}}^3}$$

$$\therefore \Delta G_V = \left(\frac{32\pi \times \gamma_{gr}^3}{3V_{gr}\, n^*} \right)^{1/3} = \left(\frac{32\pi \times (3.1\,J/m^2)^3}{3(8\times10^{-30}\,m^3/atom) \times (100\,atom)} \right)^{1/3}$$

$$= 1.08 \times 10^{10}\,J/m^3$$

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

1) $\Delta G_{v,dia}$ 구하기

$\Delta G_{v,dia} V_{dia} = {}^{\circ}G_v - {}^{\circ}G_{dia}$, $\Delta G_{v,gr} V_{gr} = {}^{\circ}G_v - {}^{\circ}G_{gr}$

$\Delta G_{v,dia} V_{dia} = \Delta G_{v,gr} V_{gr} + {}^{\circ}G_{gr} - {}^{\circ}G_{dia} = \Delta G_{v,gr} V_{gr} - 0.02 \times 1.6 \times 10^{-19}\,J/atom$

graphite의 $n^* = 100$ 일때, (e처럼)

$$\Delta G_{v,dia} = \frac{(1.08\times10^{10}\,J/m^3) \times (8\times10^{-30}\,m^3/atom) - 0.02\times1.6\times10^{-19}\,J/atom}{6\times10^{-30}\,m^3/atom}$$

$$\simeq 1.39 \times 10^{10}\,J/m^3$$

2). ΔG_{gr}^* 와 ΔG_{dia}^* 구하기

$$\Delta G_{gr}^* = \frac{16\pi \gamma_{gr}^3}{3\Delta G_{v,gr}^2} = \frac{16\pi (3.1\,J/m^2)^3}{3 \times (1.08\times10^{10}\,J/m^3)^2} = 4.28\times10^{-18}\,J$$

$$\Delta G_{dia}^* = \frac{16\pi \gamma_{dia}^3}{3\Delta G_{v,dia}^2}$$

a) $\gamma_{dia} = 3.6\,J/m^2$

$$\Delta G_{dia}^* = \frac{16\pi (3.6)^3}{3 \times (1.39\times10^{10})^2}\,J = 4.04\times10^{-18}\,J$$

b) $\gamma_{dia} = 3.65\,J/m^2$

$$\Delta G_{dia}^* = \frac{16\pi (3.65)^3}{3\times(1.39\times10^{10})^2}\,J = 4.22\times10^{-18}\,J$$

c) $\gamma_{dia} = 3.7\,J/m^2$

$$\Delta G_{dia}^* = \frac{16\pi (3.7)^3}{3\times(1.39\times10^{10})^2}\,J = 4.39\times10^{-18}\,J$$

$T = 300k$ 일때 (k는 $1.38\times10^{-23}\,J/K$)

$$\frac{I_{gra}}{I_{dia}} = \exp\left(\frac{\Delta G_{dia}^* - \Delta G_{gr}^*}{kT}\right)$$

1. $\gamma_{dia} = 3.6\,J/m^2$

$$\exp\left(\frac{(4.04-4.28)\times10^{-18}}{300\times1.38\times10^{-23}}\right) = 6.66\times10^{-26}$$

2) $\gamma_{dia} = 3.65\,J/m^2$

$$\exp\left(\frac{(4.22-4.28)\times10^{-18}}{300\times1.38\times10^{-23}}\right) = 5.08\times10^{-7}$$

3) $\gamma_{dia} = 3.7\,J/m^2$

$$\exp\left(\frac{(4.39-4.28)\times10^{-18}}{300\times1.38\times10^{-23}}\right) = 3.46\times10^{11}$$

(g) bulk에서는 graphite가 diamond 보다 안정하다. 하지만 입자의 크기가 매우 작은 경우 표면 에너지가 조금 변하도 nucleation rate이나 안정성이 매우 달라질수 있다. 따라서 diamond가 graphite 보다 nucleation이 더 잘 일어 날수 있게 된다.