1. Volume $= n\nu = \frac{4}{3}\pi r^3$

$$r^3 = \frac{3}{4}n\nu \times \frac{1}{\pi} \rightarrow r^2 = \left(\frac{3n\nu}{4\pi}\right)^{\frac{2}{3}}$$

$$\Delta G = -n\nu\Delta G_V + 4\pi r^2\gamma$$

$$= -n\nu\Delta G_V + 4\pi\left(\frac{3n\nu}{4\pi}\right)^{\frac{2}{3}}\gamma$$

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

2. (a)

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

(b)

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

$$n^* = \frac{36\pi\gamma^3}{\Delta G_V^3\,\nu}\times\frac{8}{27} = \frac{32\pi\gamma^3}{3\nu\Delta G_V^3}$$

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

$$= -\frac{32\pi\gamma^3}{3\Delta G_V^2} + 16\pi\frac{\gamma^3}{\Delta G_V^2} = \frac{16\pi\gamma^3}{3\Delta G_V^2}$$

(c)

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

$$\Delta G_{n,gra} = -n(\Delta G_{gas} - \Delta G_{gra}) + (36\pi)^{\frac{1}{3}} n^{\frac{2}{3}} V_{gra}^{\frac{2}{3}} \gamma_{gra}.$$

$$\Delta G_{n,dia} = \Delta G_{n,gra}.$$

$$n(G^{\circ}_{dia} - G^{\circ}_{gra}) = n^{\frac{2}{3}} \times (36\pi)^{\frac{1}{3}} \times (V_{gra}^{\frac{2}{3}} \gamma_{gra} - V_{dia}^{\frac{2}{3}} \gamma_{dia})$$

$$n = 36\pi \times \left(\frac{V_{gra}^{\frac{2}{3}} \cdot \gamma_{gra} - V_{dia}^{\frac{2}{3}} \gamma_{dia}}{G^{\circ}_{dia} - G^{\circ}_{gra}.} \right)^3$$

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

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

$$= 464$$

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

$$n = 145$$

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

$$n = 21$$

(d) $\Delta G_{n,gra} > \Delta G_{n,dia}$

$$-n(\Delta G_{gas} - \Delta G_{gra}) + (36\pi)^{\frac{1}{3}} n^{\frac{2}{3}} V_{gra}^{\frac{2}{3}} \gamma_{gra}$$

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

$$n(G^\circ_{dia} - G^\circ_{gra}) < n^{\frac{2}{3}} (36\pi)^{\frac{1}{3}} (V_{gra}^{\frac{2}{3}} \gamma_{gra} - V_{dia}^{\frac{2}{3}} \gamma_{dia})$$

$$n < 36\pi \times \left(\frac{V_{gra}^{\frac{2}{3}} \gamma_{gra} - V_{dia}^{\frac{2}{3}} \gamma_{dia}}{G^\circ_{dia} - G^\circ_{gra}} \right)^3$$

(e) $n^* = 100$.

$$n^* = \frac{32\pi \gamma_{gra}^3}{3 V_{gra} \Delta G_{V,gra}^3}$$

$$\Delta G_{V,gra} = \gamma_{gra} \left(\frac{32\pi}{3 n^* V_{gra}} \right)^{\frac{1}{3}}$$

$$= 3.1 \times \left(\frac{32\pi}{3 \times 100 \times 8 \times 10^{-30}} \right)^{\frac{1}{3}}$$

$$= 1.0 \times 10^{10} \ J/m^3$$

(f) $$\Delta G^* = \frac{16}{3}\pi \frac{\gamma^3}{\Delta G_V^2}$$

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

$$= \exp\left(\frac{\Delta G^*_{dia} - \Delta G^*_{gra}}{kT}\right) = \exp\left(\frac{16\pi}{3kT} \times \left(\frac{\gamma^3_{dia}}{\Delta G^2_{V,dia}} - \frac{\gamma^3_{gra}}{\Delta G^2_{V,gra}}\right)\right)$$

$$G^\circ_{dia} - G^\circ_{gra} = V_{gra}\Delta G_{V,gra} - V_{dia}\Delta G_{V,dia}$$

$$\Delta G_{V,dia} = \frac{V_{gra}\Delta G_{V,gra} - (G^\circ_{dia} - G^\circ_{gra})}{V_{dia}}.$$

$$= \frac{8\times10^{-30} \times 1.077\times10^{10} - 0.02\times1.602\times10^{-19}}{6\times10^{-30}}$$

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

if) $\gamma_{dia} = 3.6 \ J/m^2$ & $T = 300 \ k$

$$\frac{I_{gra}}{I_{dia}} = \exp\left(\frac{16\pi}{3\times1.38\times10^{-23}\times300} \times \left(\frac{3.6^3}{(1.38\times10^{10})^2} - \frac{3.1^3}{(1.077\times10^{10})^2}\right)\right)$$

$$= 1.52 \times 10^{-21}$$

if) $\gamma_{dia} = 3.65 \ J/m^2 \Rightarrow 2.37\times10^{-3}$

if) $\gamma_{dia} = 3.7 \ J/m^2 \Rightarrow 1.18\times10^{16}$

(g) Bulk 상태에서는 diamond가 graphite에 비해 불안정하지만 매우 작은 nano size에서는 diamond가 graphite보다 안정해질 수 있으며 surface energy에 매우 민감하다. 따라서 nano size에서 surface energy를 control 할 수 있다면 diamond를 얻기 용이할 것으로 생각된다.

(h) $CH_4 \rightarrow C + 2H_2$ 가 활발히 일어난다면 C의 분압이 높아지면서 size가 큰 Carbon cluster가 많이 형성되어 graphite가 생성되기 용이한 환경이 조성된다. 따라서 (e)에서 구한 graphite nucleation의 driving force는 높은 Carbon의 분압이다.