1 Nucleus의 부피를 나타낼 때, $\frac{4}{3}\pi r^3 = nv$ 로 나타낼 수 있다

이때 n은 number of atoms, v는 atomic volume을 의미한다

기존의 ΔG 식을 정리하면

$\Delta G = -\frac{4}{3}\pi r^3 \Delta G_v + 4\pi r^2 \gamma$ 이다

이 식을 위의 관계식을 이용하여 n과 v에 대한 식으로 정리하면,

$\Delta G = -nv\Delta G_v + (36\pi)^{\frac{1}{3}} n^{\frac{2}{3}} v^{\frac{2}{3}} \gamma$ 이다.

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

n = number of molecules in cluster

v = molecular volume.

(b) $\left.\frac{\partial \Delta G}{\partial n}\right)_{n=n^*} = 0$ 인 $n=n^*$를 구하면

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

$\rightarrow n^* = \frac{32\pi}{3v}\left(\frac{\gamma}{\Delta G_v}\right)^3$

$\rightarrow \Delta G(n^*) = \Delta G^* = \frac{16\pi\cdot\gamma^3}{3\cdot \Delta G_v^2}$

(c) $\Delta G = -n\cdot v\cdot \Delta G_v + (36\pi)^{\frac{1}{3}}\cdot n^{\frac{2}{3}}\cdot v^{\frac{2}{3}}\cdot \gamma$

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

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

① = ② (same stability)

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

$(36\pi)^{\frac{1}{3}}\cdot n^{\frac{2}{3}}\cdot\left\{V_{dia}^{\frac{2}{3}}\cdot\gamma_{dia} - V_{gr}^{\frac{2}{3}}\cdot\gamma_{gr}\right\} = n\cdot\left\{V_{dia}\cdot \Delta G_{v,dia} - V_{gr}\cdot \Delta G_{v,gr}\right\}$

$= n\cdot\left({}^{\circ}G_{gr} - {}^{\circ}G_{dia}\right)$

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

$\gamma_{dia} = 3.6\ J/m^2 \rightarrow n = (36\pi)\cdot\left(\frac{(6\times10^{-30}\ m^3/atom)^{\frac{2}{3}}\cdot(3.6\ J/m^2) - (8\times10^{-30}\ m^3/atom)^{\frac{2}{3}}\cdot(3.1\ J/m^2)}{-3.2\times10^{-21}\ J/atom}\right)^3 = 464$

$\gamma_{dia} = 3.65\ J/m^2 \rightarrow n = 145$

$\gamma_{dia} = 3.7\ J/m^2 \rightarrow n = 21$

(d) ~~size에 상관없이~~ diamond cluster가 graphite보다 안정하기 위해서는

$\Delta G_{dia} < \Delta G_{gr}$ 조건을 만족해야한다.

(e) $n^* = \frac{32\pi}{3v}\left(\frac{\gamma}{\Delta G_v}\right)^3$, $n^* = 100$, $V = 8\times10^{-30}\ m^3/atom$, $\gamma = 3.1\ J/m^2$.

$\Delta G_v = \gamma\cdot\left(\frac{32\pi}{3vn^*}\right)^{\frac{1}{3}} = (3.1\ J/m^2)\times\left(\frac{32\pi}{3\times(8\times10^{-30}\ m^3/atom)\times100\ atom}\right)^{\frac{1}{3}} = 1.076\times10^{10}\ J/m^3$

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

$$= \exp\left\{\frac{1}{kT}\left(\frac{16\pi}{3}\cdot\frac{\gamma_{gr}^3}{\Delta G_{v,gr}^2} + \frac{16\pi}{3}\cdot\frac{\gamma_{dia}^3}{\Delta G_{v,dia}^2}\right)\right\}$$

$$= \exp\left\{\frac{16\pi}{3\times(1.38\times10^{-23}J/K)\times298K}\left(\frac{\gamma_{gr}^3}{\Delta G_{v,gr}^2} + \frac{\gamma_{dia}^3}{\Delta G_{v,dia}^2}\right)\right\}$$

$$= \exp\left\{\frac{16\pi}{3\times(1.38\times10^{-23})\times298}\times\left(\frac{\gamma_{dia}^3}{(1.38\times10^{10})^2} - \frac{(3.1)^3}{(1.07\times10^{10})^2}\right)\right\}$$

$$\left(\because \Delta G_{v,dia} = \frac{V_{gr}\cdot\Delta G_{v,gr} - 3.2\times10^{-21}J/atom}{6\times10^{-30}m^3/atom} = \frac{(8\times10^{-30}m^3/atom)(1.076\times10^{10}J/m^3) - 3.2\times10^{-21}}{6\times10^{-30}m^3/atom} = 1.38\times10^{10}J/m^3\right)$$

i) $\gamma_{dia} = 3.6 J/m^2 \rightarrow \frac{I_{gr}}{I_{dia}} = 2.88\times10^{-27}$

ii) $\gamma_{dia} = 3.65 J/m^2 \rightarrow I_{gr}/I_{dia} = 1.42\times10^{-9}$

iii) $\gamma_{dia} = 3.7 J/m^2 \rightarrow I_{gr}/I_{dia} = 4.11\times10^{10}$

(g) diamond의 surface energy 에 따라 nucleation rate 의 차이가 크다.
surface energy가 작아질수록 좀 더 안정해진다.

(h) $CH_4 \rightarrow C + 2H_2$
위의 분해반응으로 C가 발생하는데 이 C로 cluster가 생성되는 경우 Capillary effect를 넣어 diamond 보다 graphite가 더 안정해지게 되어 최종적으로 graphite가 증착된다.