1. $V_{tot} = n \cdot v = \frac{4\pi r^3}{3}$

$\Rightarrow r^3 = \frac{3}{4\pi} n \cdot v \Rightarrow r = \left(\frac{3}{4\pi} n \cdot v\right)^{\frac{1}{3}} \Rightarrow A_{tot} = 4\pi r^2 = 4\pi \left(\frac{3}{4\pi} \cdot n \cdot v\right)^{\frac{2}{3}}$

$\therefore G_{tot} = -V_{tot} \cdot \Delta G_v + A_{tot} \cdot \gamma$

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

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

$\Rightarrow \Delta G_{tot} = -n \cdot v \, \Delta G_v + (36\pi)^{\frac{1}{3}} \cdot n^{\frac{2}{3}} \cdot v^{\frac{2}{3}} \gamma.$

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

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

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

$\Rightarrow n^{-\frac{1}{3}} = \frac{3}{2} \frac{v \cdot \Delta G_v}{(36\pi)^{\frac{1}{3}} \cdot \gamma \cdot v^{\frac{2}{3}}} \Rightarrow n^* = \frac{8}{27} \frac{36\pi \cdot v^{-3} (\Delta G_v)^{-3}}{\gamma^{-3} \cdot v^{-2}} = \frac{32\pi \gamma^3}{3 \cdot v \cdot (\Delta G_v)^3}$

$$\therefore n^* = \frac{32\pi \gamma^3}{3 \cdot v \cdot (\Delta G_v)^3}$$ //

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

$= -\frac{32\pi \cdot \gamma^3}{3 \cdot (\Delta G_v)^2} + \frac{\gamma}{\Delta G_v^2} \times 16\pi = \frac{16 \cdot \pi \cdot \gamma^3}{3(\Delta G_v)^2}$

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

(c):

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

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

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

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

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

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

① $\gamma_{dia} = 3.6\,\mathrm{J\,m^{-2}}$

$$= \frac{3.6 \times 6.242 \times 10^{18}\,\mathrm{eV}}{10^{20}\,\mathrm{\mathring{A}^{2}}}$$

$$= 0.2247\,\mathrm{eV \cdot \mathring{A}^{-2}}$$

$\gamma_{gr} = 3.1\,\mathrm{J\,m^{-2}}$

$$= 0.1935\,\mathrm{eV \cdot \mathring{A}^{-2}}$$

$$\Rightarrow n = 36\pi \left(\frac{6^{\frac{2}{3}} \times 0.2247 - 8^{\frac{2}{3}} \times 0.1935}{-0.02}\right)^{3}$$

$$= 465.7 \approx 466$$

② $\gamma_{dia} = 3.65\,\mathrm{J\,m^{-2}}$

$$= 0.2278\,\mathrm{eV \cdot \mathring{A}^{-2}}$$

$$\Rightarrow n = 36\pi \left(\frac{6^{\frac{2}{3}} \times 0.2278 - 8^{\frac{2}{3}} \times 0.1935}{-0.02}\right)^{3}$$

$$= 146.8 \approx 147$$

③ $\gamma_{dia} = 3.7\,\mathrm{J\,m^{-2}}$

$$= 0.2309\,\mathrm{eV \cdot \mathring{A}^{-2}}$$

$$\Rightarrow n = 36\pi \left(\frac{6^{\frac{2}{3}} \times 0.2309 - 8^{\frac{2}{3}} \times 0.1935}{-0.02}\right)^{3}$$

$$= 21.98 \approx 22$$

(d): $\Delta G_{dia} < \Delta G_{gr}$

$$\Rightarrow \boxed{n < 36\pi \left(\frac{V_{gr}^{\frac{2}{3}} \cdot \gamma_{gr} - V_{dia}^{\frac{2}{3}} \cdot \gamma_{dia}}{{}^\circ G_{T\,dia} - {}^\circ G_{T\,gr}}\right)^3}$$

(e):

$$n^* = \frac{32\pi \cdot \gamma_{gr}^3}{3 \cdot V_{gr} \cdot (\Delta G_{v})^3} = \frac{32\pi \times (3.1\,J\,m^{-2})^3}{3\times(8\times10^{-30}\,m^3/atom)\times(\Delta G_{v})^3} = 100$$

$$\Rightarrow (\Delta G_{v})^3 = \frac{32\pi \times (3.1\,J\,m^{-2})^3}{3\times(8\times10^{-30}\,m^3/atom)\times 100} =$$

$$(\Delta G_{v}) = \left\{\frac{32\pi \times (3.1\,J\,m^{-2})^3}{3\times8\times10^{-30}\,m^3/atom \times 100}\right\}^{\frac{1}{3}} = 1.0766\times10^{10}\,J\,m^{-3}$$

$$\boxed{\therefore \Delta G_v^{gr} = 1.0766\times10^{10}\,J\,m^{-3}}$$

(f):

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

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

$\boxed{\Delta G_v^{dia}}$

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

$$\Rightarrow \Delta G_v^{dia} = \frac{V_{gr}\Delta G_v^{gr} - ({}^\circ G_{dia} - {}^\circ G_{gr})}{V_{dia}} = \frac{8\times10^{-30}\times1.0766\times10^{10} - 0.02\times1.602\times10^{-19}}{6\times10^{-30}}$$

$$= 1.3820\times10^{10}\,J\,m^{-3}$$

$$\boxed{\therefore \Delta G_v^{dia} = 1.3820\times10^{10}\,J\,m^{-3}}$$

① $\Gamma_{dia} = 3.6\,Jm^{-2}$

$$\frac{I_{gr}}{I_{dia}} = \exp\left\{ \frac{16\pi}{3\times1.38\times10^{-23}\times298K} \left(\frac{(3.6)^3}{(1.3620\times10^{10})^2} - \frac{(3.1)^3}{(1.0766\times10^{10})^2} \right) \right\}$$

$$= \exp\left\{ 4.074\times10^{21} \left(\quad \text{''} \quad \right) \right\}$$

$$= \boxed{2.83\times10^{-23}}$$

② $\Gamma_{dia} = 3.65\,Jm^{-2}$

$$\Rightarrow \boxed{5.16\times10^{-5}}$$

③ $\Gamma_{dia} = 3.7\,Jm^{-2}$

$$\Rightarrow \boxed{3.02\times10^{14}}$$

(g): (c)를 통해 diamond는 bulk state이 아닌 nano size가 작을 때 비로소 graphite보다 stability가 높아지고 (f)를 통해 diamond의 nucleation은 surface energy에 따라 매우 민감하게 달라질수 있음을 알수 있다.
즉, diamond를 이루는 cluster의 개수에 따라서 surface energy를 미세하게 control 하며 특정 surface energy (diamond)에서 diamond의 nucleation을 증대시킬수 있다.

(h): $CH_4 \rightarrow C + 2H_2$ 의 decomposition 반응을 촉진시킴에 따라서 Carbon의 partial pressure가 증가하게 된다. 분해된 Carbon gas는 graphite로 응축되어지기에 (e)에서의 ΔG_v는 감소할 것이다. 즉, graphite nucleation의 driving force는 Carbon의 partial pressure이다.