

AMSE502 Phase Transformations

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Problem Set #5

Prof. Byeong-Joo Lee
 calphad@postech.ac.kr
 Room 1- 311

1. Assuming a spherical nucleus, derive the following expression for the nucleation energy.

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

where n is number of atoms and ν is atomic volume.

2. (Nucleation Kinetics of CVD Diamond) Diamond is a less stable form of carbon than graphite, but it can be obtained by CVD under normal pressure and temperature.

- For a spherical nucleus, express the energy change during nucleation as a function of number of atoms in cluster.
- Using the result of (a), derive the expression for the critical number of atoms and energy barrier.
- Assuming isotropic and constant surface energy for both of graphite and diamond, and using the data : $\gamma_{gr} = 3.1 \text{ Jm}^{-2}$, $\gamma_{dia} = 3.6, 3.65 \text{ and } 3.7 \text{ Jm}^{-2}$, respectively
 $v_{gr} = 8 \text{ \AA}^3/\text{atom}$, $v_{dia} = 6 \text{ \AA}^3/\text{atom}$, ${}^{\circ}G_{dia} - {}^{\circ}G_{gr} = 0.02 \text{ eV/atom}$

For the three slightly different values of surface energy of diamond, compute the number of atoms in clusters where the stability of diamond becomes the same as that of graphite.

- What is the necessary condition for a diamond cluster of any size to be more stable than graphite ?
- Assuming that the critical number of atoms for graphite nucleation is 100, estimate the driving force for graphite nucleation.
- For the three values of surface energy of diamond, compute the ratio of nucleation rate between graphite and diamond, I_{gra}/I_{dia} .
 For the nucleation rate, use the expression: $I = A \cdot \exp(-\Delta G^*/kT)$, and assume that A is the same constant for both of graphite and diamond.
- What is your conclusion on this problem?
- Suppose that the source of carbon in the CVD is the decomposition of CH_4 into C and H_2 .

$$\text{CH}_4 \rightarrow \text{C} + 2\text{H}_2$$
 If the C was deposited as graphite, what would be the physical meaning of driving force of graphite nucleation [the value you obtained in e)] ?