Department of Materials Science and Engineering
Pohang University of Science and Technology

AMSE502 Phase Transformations

due Date: May 11, 2023

Problem Set #5

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

1. (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. (27)

a) For a spherical nucleus, derive the following expression, the energy change during nucleation as a function of number of atoms *n* in cluster (*v* is atomic volume).

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

b) Using the result of (a), derive the expression for the critical number of atoms and energy barrier.

c) Assuming isotropic and constant surface energy for both of graphite and diamond, and using the data : γ_{gr} = 3.1 Jm^{-2}, γ_{dia} = 3.6, 3.65 and 3.7 Jm^{-2}, respectively
v_{gr} = 8 $Å^3$/atom, v_{dia} = 6 $Å^3$ /atom, $^oG_{dia}$ - $^oG_{gr}$ = 0.02 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.

d) What is the necessary condition for a diamond cluster of any size to be more stable than graphite ?

e) Assuming that the critical number of atoms for graphite nucleation is 100, estimate the driving force for graphite nucleation.

f) 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 and T = 300 K.

g) What is your conclusion on this problem?