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

AMSE502 Phase Transformations

due Date: Nov. 8, 2016

Problem Set #3

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Room 1- 311

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

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

where n is number of atoms and v 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.

a) For a spherical nucleus, express the energy change during nucleation as a function of number of atoms in cluster.

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 : $\gamma_{gr} = 3.1$ Jm^{-2}, $\gamma_{dia} = 3.6$, 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.

g) What is your conclusion on this problem?

h) Suppose that the source of carbon in the CVD is the decomposition of CH_4 into C and H_2.

$$CH_4 \rightarrow C + 2H_2.$$

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)] ?

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3. Read the following papers and summarize on one PPT slide

- Prediction of Interface Reaction Products between Cu and Various Solder Alloys by Thermodynamic Calculation
  Byeong-Joo Lee, N.M. Hwang and H.M. Lee, Acta Materialia 45, 1867-1874 (1997).
- Prediction of Ti/Al2O3 Interface Reaction Products by Thermodynamic Calculation
  Byeong-Joo Lee, J. Korean Institute of Metals & Materials 34, 864-869 (1996).
- Prediction of Ti/Al2O3 Interface Reaction Products by Diffusion Simulation
  Byeong-Joo Lee, Acta Materialia 45, 3993-3999 (1997).
- Thermodynamic Analysis of Solid State Metal/Si Interfacial Reactions
  Byeong-Joo Lee, J. Materials Research 14, 1002-1017 (1999).