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



**AMSE502 Phase Transformations**

due Date: Oct. 07, 2014 Prof. Byeong-Joo Lee

Problem Set #1

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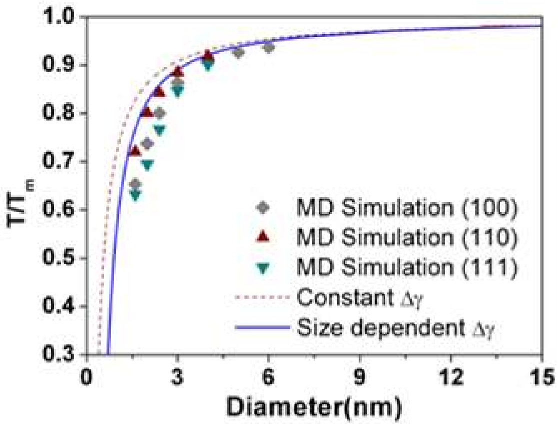
Room 1- 311

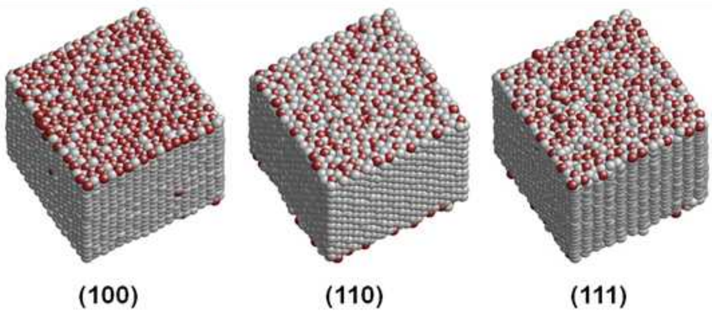
1. The fcc Fe-M-C ternary solid solution phase can be described using a two sublattice model with a formula unit, $(Fe,M)_a(Va,C)_c$.
   (a) Write the expression for the Gibbs free energy of this phase per mole of formula unit, using a regular solution model for each binary (use one L parameter for the excess energy term).
   (b) Derive an expression for the chemical potential of carbon.

2. The following figure shows molecular dynamics simulations for the drop of melting point of Ni nanowires. (100) means the cross sectional plane of the wire or the <100> direction of wire axis.
   (a) Derive an expression for the melting point drop due to the capillary effect for nanowires.
   (b) Explain the reason why the degree of melting point drop changes depending on the direction of wire axis.




3. Among the three low index surfaces, (100), (110) and (111), the (110) surface is the lowest energy surface for bcc metals. The followings show the change of surface energy due to surface segregation of impurity atoms (red spheres) for bcc Fe. Try to explain why the surface energy of (100) could become lower than the (110) surface energy after the surface segregation.

| Surface | Bulk Concentration | Ave. Concentration within a unit cell distance from surface | Surface E, J/m$^2$ |
|---|---|---|---|
| (100) | 0.01% | 30% | 0.80 |
| (110) | 0.01% | 12% | 1.61 |
| (111) | 0.01% | 27% | 1.43 |
| $E_{surf\ of\ pure\ Fe}$ = 2.50, 2.35, 2.56 for (100), (110), (111) | | | |



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4. Study and summarize CSL(coincidence site lattice) boundary.

5. Assuming a one atomic layer surface phase and considering equilibrium between bulk and surface phases, one can derive the following relation between surface composition and bulk composition. (B means "bulk" and $\phi$ means "surface". *i* means arbitrary solute elements while *n* means solvent element)

$$\frac{X_i^\phi}{X_n^\phi} = \frac{X_i^B}{X_n^B}\ e^{-\Delta G^{seg}/RT} \quad \text{where} \qquad \Delta G^{seg} = [{}^oG_i^\phi - {}^oG_i^B] - [{}^oG_n^\phi - {}^oG_n^B] + RT\ln\frac{\gamma_i^\phi \gamma_n^B}{\gamma_n^\phi \gamma_i^B}$$

Change the above equation into the following, more general multicomponent form:

$$X_i^\phi = \frac{X_i^B e^{-\Delta G_i^{seg}/RT}}{1+\sum_{j=1}^{n-1} X_j^B (e^{-\Delta G_j^{seg}/RT} - 1)} \qquad \text{Hint: use } \sum_{i=1}^{n-1} x_i^\phi x_n^B = \sum_{j=1}^{n-1} x_j^B x_n^\phi\ e^{-\Delta G_j^{seg}/RT}$$