MSE 301 Integrated Computational Materials Engineering
Homework 3: Phase Field Modeling
Due in class on Thursday April 23

A. Conceptual Short Answer Questions: (30 points, 5 points each)

1. What are the differences between sharp-interface models and phase field models?
2. What are the differences between first and second order transformations and their order parameters?
3. What are the differences between phase field and phase field crystal models?
4. What numerical methods can be used to solve governing equations of phase field models? (name three methods)
5. What model parameters or materials properties control the interface thickness of phase field models (Model A and Model B)?
6. Consider that in a system two different phenomena are happening (for example nano-particle precipitation and grain boundary movement), one is at nanoscale (50-100 nm) and another one is at microscale (5-20 micron), and the goal is to simulate their evolutions and interactions. What are your suggestions in developing a phase field model for such a system?

B. Calculation: (20 points total)

Consider Ginzburg-Landau equation at equilibrium, order parameter ϕ, and a double-well potential which takes value zero at $\phi = -1$ and $\phi = 1$ for Landau free energy density, determine the interface thickness of the phase field model when the height of the energy barrier is *H* and gradient energy coefficient is *K*.

C. Simulations: (50 points)

1. Phase transitions with a symmetric phase diagram (20 points)

Consider the example in PFM lecture-1 (page 21), introduce anisotropy to the system by assuming W_0 is a function of the angle of the local interface normal: $W_0 = \overline{W}(1+\varepsilon\cos(n\theta))$, $\overline{W} = 1$. Simulate the microstructural evolution in COMSOL and plot the results at *t*=500 for n=2 and different values of ε (= 0, 0.1,0.2).

2. <u>Thin film growth simulations:</u> (30 points)

Consider a binary system, with components A and B, which forms up to three phases (α, β, and γ), and characterized by the molar fraction of the component B, *c*. The Landau free energy density of a uniform unstressed system is assumed to be a triple well potential that can produce two-phase and three-phase binary systems:

$f(c) = W_1(c-c^\alpha)^2(c-c^\beta)^2(c-c^\gamma)^2 + W_2(c-c^\alpha)^2(c-c^\gamma)^2$. For non-dimensional simulations assume that scaled composition c varies between $c^\alpha = -1$ and $c^\gamma = 1$, with intermediate phase at $c^\beta = 0$, and $W_1 = 0.4$, $W_2 = -0.04$ (which produces a stable intermediate phase). Use the Cahn-Hilliard equation and assume that non-dimensional gradient energy coefficient and mobility take value unity.

1. <u>1D simulations-thin film diffusion couple</u>: Choose a100 non-dimensional length domain, and for initial condition put $c^\alpha = -1$ for one half of the domain and $c^\gamma = 1$ for the other half of the domain. Use no-flux boundary condition. Simulate the growth of an intermediate thin film growth in COMSOL. Vary the mesh size to find the coarsest mesh size for convergence to the right answer by plotting the intermediate phase thickness versus evolution time.
2. <u>2D simulations-thin film diffusion couple</u>: Use a 100 by 50 non-dimensional domain size; for initial condition put $c^\alpha = -1$ for one half of the domain and $c^\gamma = 1$ for the other half of the domain. Use periodic boundary in the interface direction and no-flux perpendicular to the interface direction. Use mapped mesh (square) with the element size calculate from 1D simulations. Simulate the growth of an intermediate thin film growth in COMSOL. Plot the intermediate phase thickness versus evolution time and compare the result to 1D simulation.