MM-640 Midsem Project

Preliminary Presentation

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Phase field study of grain boundary effects on spinodal decomposition

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Have developed a phase field model of a **polycrystalline binary alloy** by combining

1. The **Cahn–Hilliard** model for a compositionally inhomogeneous alloy
2. A model of polycrystals (Fan D, Chen L-Q. Acta Mater. 1997;45:3297) which is governed by the **Cahn–Allen** equation for non-conserved variables

Have used this model to study **grain boundary (GB)** effects on **spinodal decomposition (SD)** in two-dimensional (2D) systems.

I. Model

I.1. Cahn Hilliard Model

Cahn–Hilliard Model for a compositionally inhomogeneous alloy is used. It is developed using the composition field **c(r)** in an alloy.

The local composition **c** used in this model is defined as follows:

$$c = \frac{c' - c'_\alpha}{c'_\beta - c'_\alpha}$$

where, c' is the local composition,

c'_α is the equilibrium composition of A rich α phase,

c'_β is the equilibrium composition of B rich β phase

I.1. Cahn Hilliard Model (contd.)

$$c = \frac{c' - c'_\alpha}{c'_\beta - c'_\alpha}$$

where, c' is the local composition,

c'_α is the equilibrium composition of A rich α phase,

c'_β is the equilibrium composition of B rich β phase

all the values are expressed in mole fraction of species B. Thus, for **α phase c = 0** and for **β phase c = 1**

I.2. Cahn Allen Model

Cahn–Allen theory for non-conserved variables (the model of Fan and Chen (1997) belongs to this category) is used. It is developed using a set of n 'orientational' (and non-conserved) order parameter fields $\eta_i(r)$ (i = 1,2,…,n) to represent n different grain orientations in the microstructure; η_i are continuum analogues of Potts variables in the n-state Potts model

I.2. Cahn Allen Model (contd.)

Each η_i is taken to be **1** within the **ith** grain and drops to **0** outside it, through a GB region where it varies smoothly.

The schematic profiles of two orientation variables across a flat grain boundary.
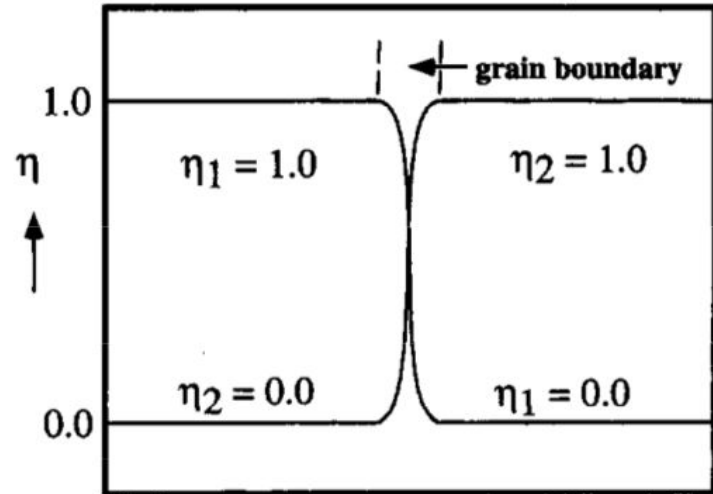
I.3. Conclusion

An instantaneous configuration in our model is described in terms of the **n+1** position-dependent field variables **$(c; \eta_1, \eta_2, \ldots\ldots, \eta_n)$**.

II. Mathematical Formulation of the Model

II.1. Energetics

The Total Free energy, **F**, of a system with inhomogeneities in both **c** and **η$_i$** is written as a volume integral:

$$F = N_V \int \left[f(c, \eta_i) \ + \ \kappa_c (\nabla c)^2 \ + \ \sum_i^n \kappa_i (\nabla \eta_i)^2 \right]$$

II.1. Energetics (contd.)

$$F = N_V \int \left[f(c, \eta_i) \ + \ \kappa_c (\nabla c)^2 \ + \ \sum_i^n \kappa_i (\nabla \eta_i)^2 \right]$$

where
N_V is the (constant) number of atoms per unit volume,
$f(c, \eta_i)$ is the bulk free energy density and,
κ_c & κ_i are the (constant) gradient energy coefficients associated with inhomogeneities in c and in η_i, respectively.
It is assumed that $\kappa_i = \kappa_\eta$ for all i.

II.1. Energetics (contd.)

Thus, the bulk free energy density $f(c,\eta_i)$ is chosen such that it exhibits a minimum for these **2n** possibilities. In other words, **f** has **2n degenerate minima** (whose value is chosen to be **0**)

These minima are located at **n** grains of **α** with a composition of **c = 0**:

(0;1,0,...,0), (0;0,1,...,0),...,(0;0,0,...,1),

and **n** grains of **β** with a composition of **c = 1**:

(1;1,0,...,0), (1;0,1,...,0),...,(1;0,0,...,1).

II.1. Energetics (contd.)

$$f(c,\eta_i)=f(c_o)+m(c)\left\{0.25+\sum_i^n\left[-\frac{\eta_i^2}{2}+\frac{\eta_i^4}{4}\right]+\varepsilon\sum_i^n\sum_{j>i}^n\eta_i^2\eta_j^2\right\}$$

$f_o(c)$ is the free energy per atom in a bulk single crystal of composition **c** given by:

$$f(c_o)=A_c c^2(1-c)^2$$

II.1. Energetics (contd.)

$$f(c_o) = A_c c^2 (1-c)^2$$

The constant A_c determines the height of the free energy barrier between the equilibrium phases within a single grain, **m(c)** is a composition dependent factor which couples **c & η_i** and **ε** is a constant.

II.1. Energetics (contd.)

$$f(c,\eta_i)=f(c_o)+m(c)\left\{0.25+\sum_i^n\left[-\frac{\eta_i^2}{2}+\frac{\eta_i^4}{4}\right]+\varepsilon\sum_i^n\sum_{j>i}^n\eta_i^2\eta_j^2\right\}$$

Note that the terms within the curly braces are even functions of η_i ; therefore, **f(c,η_i)** has additional degenerate minima at **2n** more locations with negative values of η_i such as **{c ;η_i} = (0;-1,0,...,0),....** In this case, these extra degenerate equilibrium states are excluded by working only with η_i**>=0**.

II.2. Kinetics

The evolution of the composition field **c** is governed by the **Cahn–Hilliard equation** for conserved variables:

$$\frac{dc}{dt} = M\nabla^2\left[\frac{\delta(F/N_v)}{\delta c}\right]$$

where **$d(F/N_v)/dc=\mu$** is the chemical potential whose gradient drives diffusion, and **M** is the atomic mobility.

II.2. Kinetics (contd.)

The evolution of order parameter fields η_i is governed by the **Cahn–Allen equation** for non-conserved variables:

$$\frac{d\eta_i}{dt} = -L_i \left[\frac{\delta(F/N_V)}{\delta\eta_i} \right]$$

where $\partial(F/N_V)/\partial\eta_i$ is the total free energy (per atom) with respect to η_i, and L_i are the relaxation coefficients for η_i. Here, **M** and $L_i = L$ **(i = 1,2,…,n)** are assumed to be constants.

II.3. Numerical Implementation

$$\frac{dc}{dt} = M\nabla^2[g(c) - 2\kappa_c\nabla^4 c]$$

where **g(c) = ∂f/∂c**

The numerical method used in our simulations is based on the **semi-implicit Fourier spectral method**

$$\tilde{c}(\mathbf{k}, t + \Delta t) = \frac{\tilde{c}(\mathbf{k}, t) - \Delta t M k^2 \tilde{g}(\mathbf{k}, t)}{1 + 2\Delta t M \kappa_c k^4},$$

II.3. Numerical Implementation (contd.)

Similarly for the **Cahn–Allen equation**

$$\tilde{\eta}_i(\mathbf{k},t + \Delta t) = \frac{\tilde{\eta}_i(\mathbf{k},t) - \Delta t L_i \tilde{\tilde{h}}_i(\mathbf{k},t)}{1 + 2\Delta t L_i \kappa_\eta k^2},$$

where $\mathbf{h}_i = \partial f / \partial \mathbf{h}_i$

III. Settings for Simulation

III.1. The values of the parameters

Model parameter	Value
A	1.0
κ_c	1.0
M	1.0
ε	2.0
$\kappa_i = \kappa_\eta$	1.0
$L_i = L$	1.0
Simulation parameter	Value
$\Delta x = \Delta y$	1.0
Δt	0.1
$N_x \times N_y$	512×256 (two-grain case)
	512×512 (polycrystalline case)

III.2. Variation of m(c) & ∂_c(disturbance)

The Initial Profile is set by $c_o = 0.5 \pm \partial_c$
∂_c is varied from 0.01 to 0.04

System index	$m(c)$	κ_η
Ia	$1 + 0.5c^2$	1.0
Ib	$1 + 0.5c^2 - 2.5c^2(1-c)^2$	1.0
Ic	$2 + c^2$	0.5
IIa	$1 + 0.1c^2$	1.0

IV. Pseudo Code

Take input from file input.dat
n_x, delta_x, n_y, delta_y, T, delta_t, T_write(after how many steps do we print the output in a file)

Declare composition,n1,n2,g,h1 & h2 matrix and **Allocate memory**
Declare the **Fourier Transform's** respectively

Calculate half_nx, half_ny, delta_kx & delta_ky

Make the Initial Profile
Traverse the matrix
    Generate Random Number R=[-1,1]
    composition=0.5 +- R*0.04
            IF i<half_nx
              n1=1 & n2=0
            ELSE
            n1=0 & n2=1

Start time loop
    Traverse Matrix
        Calculate g,h1,h2
    Take composition,n1,n2,g,h1 & h2 **to Fourier space**
    Evolve composition
    Traverse Matrix
        Calculate kx,ky
        Calculate new composition,n1 & n2 --
    Take composition,n1 & n2 back **to real space**
    Traverse Matrix
    Normalise the values and **Set** imaginary part to zero for composition,n1 & n2
    After every T_write time steps **write** composition profile **to file**
end time loop

Free all memory

Thank You