

Phase field modelling of microstructural evolution using the Cahn-Hilliard equation: A report to accompany CH-muSE

1 The Cahn-Hilliard equation

Let us consider a binary alloy of average composition c_0 occupying the (2D) xy -plane. Let the alloy consist of two phases m and p , that is, it is kept at a temperature (say T) that corresponds to the two phase region in the phase diagram (see Figure 1). We assume that the temperature remains a constant, i.e., our present formulation is an isothermal one.

Let the composition at any point \mathbf{r} in the xy -plane at time t be denoted by $c(\mathbf{r}, t)$. Let the microstructure of the system be completely described by the composition field. Let us choose a domain Ω bounded by $\partial\Omega$ of such a system. Further, we assume the composition field to be periodic on Ω , i.e., Ω is the representative area for the 2-dimensional system and repeats infinitely to fill the entire xy -plane (see Figure 2). This assumption of periodicity helps us avoid accounting for the surfaces in our calculations.

Given an initial composition profile, say $c(\mathbf{r}, 0)$, the composition profile at any future time t can be obtained by solving the following (Cahn-Hilliard) non-linear diffusion equation (with periodic boundary conditions):

$$\frac{\partial c}{\partial t} = \nabla \cdot M \nabla \mu, \quad (1)$$

where, M is the mobility, c is the (scaled) composition t is the time, and μ is the chemical potential, given by

$$\mu = \frac{\delta F^{ch}}{\delta c}, \quad (2)$$

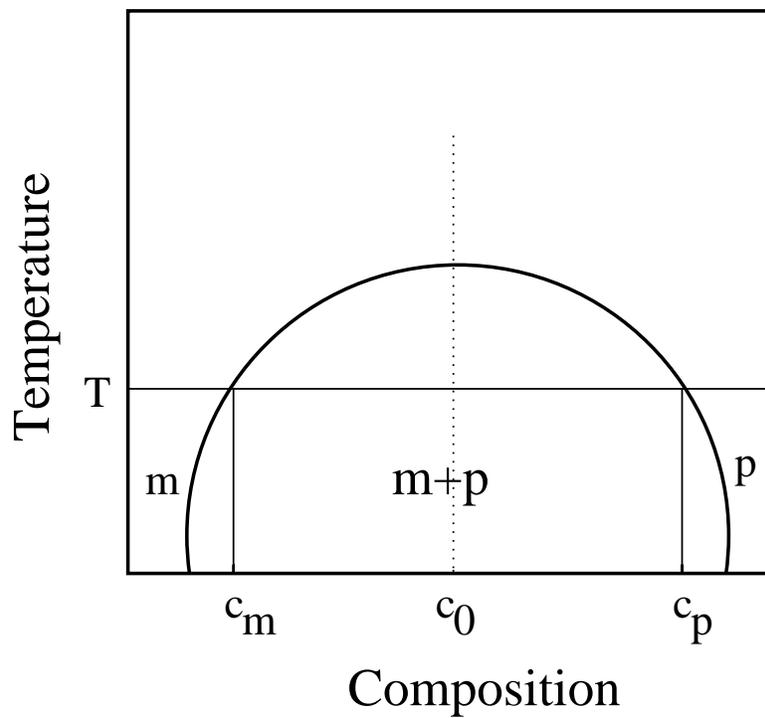


Figure 1: Schematic phase diagram.

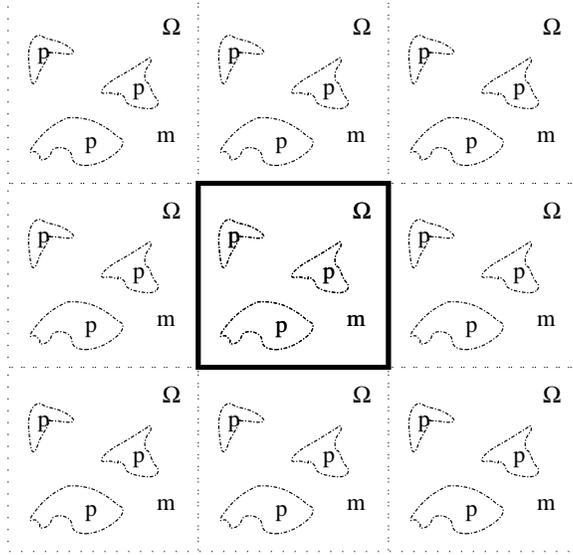


Figure 2: Periodic domain Ω .

where $\frac{\delta}{\delta c}$ denotes the variational derivative with respect to composition, and F is the chemical free energy

$$F^{ch} = N_{AV} \int_{\Omega} [f_0(c) + \kappa(\nabla c)^2] d\Omega, \quad (3)$$

where, N_{AV} is the Avogadro number, κ is the gradient energy coefficient, and $f_0(c)$ is the bulk free energy density, and is given by

$$f_0(c) = Ac^2(1 - c)^2, \quad (4)$$

where A is a positive constant indicating the energy barrier between the two equilibrium phases m and p (see Figure 3). Using the expressions (3) and (4) in the definition of the chemical potential, we obtain

$$\mu = h - 2\kappa\nabla^2 c, \quad (5)$$

where,

$$h = \frac{\partial f_0}{\partial c} = 4Ac(1 - c)(1 - 2c). \quad (6)$$

We assume the mobility M and the gradient energy κ to be (scalar) constants: this amounts to assuming the interfacial energies and the diffusivities to be isotropic.

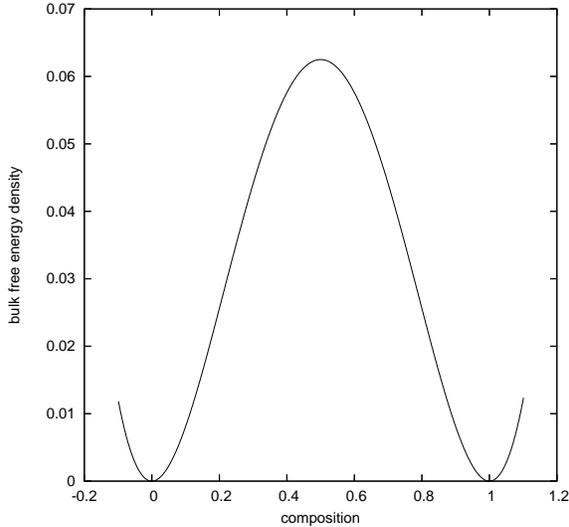


Figure 3: Bulk free energy density as a function of composition for $A=1$. Note that the energy barrier is one-sixteenth of A , and the equilibrium compositions of the m and p phases are scaled to be zero and unity respectively

Using the Equation (5) above, and the fact that M is a constant, we obtain the Cahn-Hilliard equation as follows:

$$\frac{\partial c}{\partial t} = M \nabla^2 (h - 2\kappa \nabla^2 c). \quad (7)$$

2 Numerical implementation and benchmarking

2.1 Implementation details

2.1.1 Non-dimensionalisation

All the parameters used in our simulations are non-dimensional. The non-dimensionalisation was carried out using the characteristic length L' , energy E' , and time T' , as follows:

$$L' = \left(\frac{\kappa}{A} \right)^{\frac{1}{2}}, \quad (8)$$

$$E' = AL'^3, \quad (9)$$

$$T' = \frac{L'^2(c_p^e - c_m^e)^2}{ME'}, \quad (10)$$

where c_p^e and c_m^e are the equilibrium precipitate and matrix compositions, respectively. We note that this choice of non-dimensionalisation renders the non-dimensional κ , A , and M unity.

Thus, using these non-dimensionalisation we obtain the following Cahn-Hilliard equation (from Equation (7)):

$$\frac{\partial c}{\partial t} = \nabla^2(h - 2\nabla^2 c). \quad (11)$$

2.1.2 Fourier transform and discretization

Let us consider the equation (11) above and take the (spatial-) Fourier transform on both sides of the equations:

$$\frac{\partial \{c\}_{\mathbf{g}}}{\partial t} = -g^2(\{h\}_{\mathbf{g}} + 2g^2\{c\}_{\mathbf{g}}), \quad (12)$$

where, $\{\cdot\}_{\mathbf{g}}$ represents the (spatial-) Fourier transform of the quantity $\{\cdot\}$.

The semi-implicit discretization of the above equation is then obtained as follows:

$$\frac{c(\mathbf{g}, t + \Delta t) - c(\mathbf{g}, t)}{\Delta t} = -g^2\{h\}_{\mathbf{g}} - 2g^4 c(\mathbf{g}, t + \Delta t) \quad (13)$$

$$c(\mathbf{g}, t + \Delta t) = \frac{c(\mathbf{g}, t) - g^2\{h\}_{\mathbf{g}}\Delta t}{1 + 2\Delta t g^4}, \quad (14)$$

where Δt is the time step for the numerical integration. Thus the problem of microstructural evolution reduces to numerically solving the discretized equation above.

2.1.3 Algorithm for microstructural evolution

The following is the algorithm for microstructural evolution:

1. Given a composition profile at time t , we calculate the h and its Fourier transform as well as the Fourier transform of c .
2. Using $\{h\}_{\mathbf{g}}$ and $\{c\}_{\mathbf{g}}$ in equation (14), we calculate the composition profile at some future time $t + \Delta t$.
3. The inverse Fourier transform of $c(t + \Delta t)$ gives the composition profile at time $t + \Delta t$.
4. We repeat steps 1-3 to march in time for the given number of time steps.

The (discrete) Fourier transforms needed for our calculations have been carried out using FFTW developed by Frigo and Johnson [1].

3 Acknowledgements

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References

- [1] M Frigo and SG Johnson (2005), *The design and implementation of FFTW3*, Proceedings of the IEEE, **93**, 2, p. 216. (See also <http://www.fftw.org>)

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