Series lectures of phase-field model

05. Allen-Cahn Equation

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November 21, 2024

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Derivation of Allen-Cahn equation

- The equation is

$$\mathbf{J} = -M\nabla\lambda = -M\nabla\frac{\delta F}{\delta c}$$

- For conserved field,

$$\frac{\partial c}{\partial t} = -\nabla\cdot\mathbf{J} = \nabla\cdot M\nabla\frac{\delta F}{\delta c}$$

Order parameter ϕ which is not conserved.

$$\frac{\partial\phi}{\partial t} = -L\frac{\delta F}{\delta\phi} = -L\left[\frac{\partial f}{\partial\phi} - 2\kappa\nabla^2\phi\right]$$

Analytic solution for small perturbation case

- For the case

$$f(\phi) = A\phi^2(1-\phi)^2$$

assume

$$\phi(x) = \phi_0 + \varepsilon\tilde{\phi}(x,\varepsilon)$$

$$\frac{\partial \phi}{\partial t} = \varepsilon \frac{\partial \tilde{\phi}}{\partial t} \qquad \frac{\partial^2 \phi}{\partial x^2} = \varepsilon \frac{\partial^2 \tilde{\phi}}{\partial x^2}$$

$$\frac{\partial f}{\partial \phi} = \cancelto{0}{\left.\frac{\partial f}{\partial \phi}\right|_{\phi_0}} + \left.\frac{\partial^2 f}{\partial \phi^2}\right|_{\phi_0} (\phi - \phi_0) = \varepsilon \left.\frac{\partial^2 f}{\partial \phi^2}\right|_{\phi_0} \tilde{\phi}(x,t)$$

- Using the relation above, Allen-Cahn equation becomes

$$\frac{\partial \tilde{\phi}}{\partial t} = -L\left[\left.\frac{\partial^2 f}{\partial \phi^2}\right|_{\phi_0} \tilde{\phi} - 2\kappa \frac{\partial^2 \tilde{\phi}}{\partial x^2} \right]$$

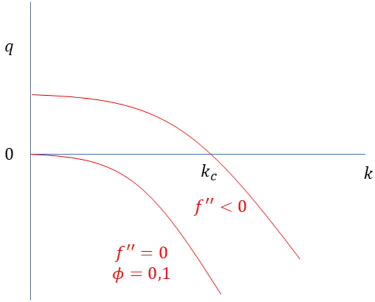
- Take Fourier transform,

$$\frac{\partial \Phi(k,t)}{\partial t} = -L\left[\left.\frac{\partial^2 f}{\partial \phi^2}\right|_{\phi_0} \Phi(k,t) + 2\kappa k^2 \Phi(k,t) \right]$$

- Let

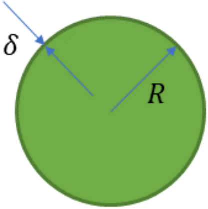
$$q = -L\left[\left.\frac{\partial^2 f}{\partial \phi^2}\right|_{\phi_0} + 2\kappa k^2 \right]$$

$$\Phi(k,t) = \Phi(k,0)e^{qt}$$

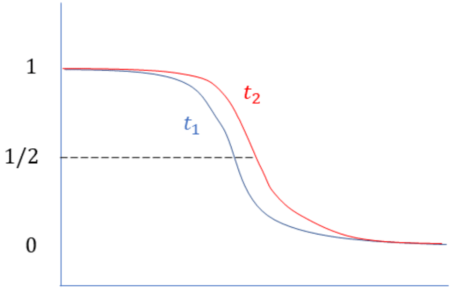


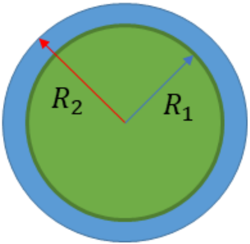
Evolution of spherical domain

- Thickness of interface, δ, mean curvature H, $\delta H \ll 1$



- Schematic drawing of profile is given as below.





- Motion of level curves of $\phi = 0.5$

$$\phi(r(t), t) = 0.5 \rightarrow \frac{d}{dt}\phi(r(t), t) = 0$$

$$\frac{d}{dt}\phi(r(t), t) = \frac{\partial \phi}{\partial r}\bigg|_t \frac{\partial r}{\partial t} + \frac{\partial \phi}{\partial t}\bigg|_r = 0 \rightarrow \frac{\partial \phi}{\partial t}\bigg|_r = -\frac{\partial \phi}{\partial r}\bigg|_t \frac{\partial r}{\partial t}$$

  we call it as level set equation.
- For a spherical particle $\phi = 1$ inside $\phi = 0$ outside.
- Allen-Cahn equation in spherical coordinates

$$\begin{aligned} \frac{\partial \phi}{\partial t} &= -L\left[\frac{\partial f}{\partial \phi} - \frac{2\kappa}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial \phi}{\partial r}\right)\right] \\ &= -L\left[\frac{\partial f}{\partial \phi} - \frac{2\kappa}{r^2}\left(2r\frac{\partial \phi}{\partial r} + r^2 \frac{\partial^2 \phi}{\partial r^2}\right)\right] \\ &= -L\left[\frac{\partial f}{\partial \phi} - \frac{4\kappa}{r}\frac{\partial \phi}{\partial r} - 2\kappa \frac{\partial^2 \phi}{\partial r^2}\right] \end{aligned}$$

- In 1-D case, Euler-Lagrange equation becomes

$$\frac{\partial f}{\partial \phi} - 2\kappa \frac{d^2\phi}{dx^2} = 0$$

Integrate with respect to ϕ

$$f(\phi) - \kappa \left(\frac{d\phi}{dx} \right)^2 = 0$$

at equilibrium.

- Assume that the interface is sufficiently planar that

$$\frac{\partial f}{\partial \phi} - \kappa \frac{\partial}{\partial \phi}\left(\frac{\partial \phi}{\partial r}\right)^2 = 0$$

assuming $\delta/R \ll 1$.

- Substitute into Allen-Cahn equation

$$\frac{1}{L}\frac{\partial \phi}{\partial t} = -\kappa \frac{\partial}{\partial \phi}\left(\frac{\partial \phi}{\partial r}\right)^2 + \frac{4\kappa}{r}\frac{\partial \phi}{\partial r} + 2\kappa \frac{\partial^2 \phi}{\partial r^2}$$

With

$$\frac{\partial}{\partial \phi}\left(\frac{\partial \phi}{\partial r}\right)^2 = \frac{\partial r}{\partial \phi}\frac{\partial}{\partial r}\left(\frac{\partial \phi}{\partial r}\right)^2 = \frac{\partial r}{\partial \phi}\left(2\frac{\partial \phi}{\partial r}\right)\frac{\partial^2 \phi}{\partial r^2} = 2\frac{\partial^2 \phi}{\partial r^2}$$

- Allen-Cahn equation becomes

$$\frac{1}{L}\frac{\partial \phi}{\partial t} = -2\kappa \cancel{\frac{\partial^2 \phi}{\partial r^2}} + \frac{4\kappa}{r}\frac{\partial \phi}{\partial r} + 2\kappa \cancel{\frac{\partial^2 \phi}{\partial r^2}}$$

- It proceeds

$$-\frac{\partial \not{\phi}}{\not{\partial} r}\frac{\partial r}{\partial t} = \frac{4\kappa L}{r}\frac{\partial \not{\phi}}{\not{\partial} r}$$

- Finally, we have

$$\frac{\partial r}{\partial t} = v = -\frac{4\kappa L}{r}$$

  where v is the velocity of the interface.

- Curvature

$$H = \frac{1}{2}\left(\frac{1}{r_1} + \frac{1}{r_2}\right) = \frac{1}{r} \quad \text{for spherical particle}$$

$$v = -4\kappa L H$$

  motion by mean curvature, grain growth in isotropic system, motion of antiphase domain boundaries.

- The rate equation is

$$\frac{\partial r}{\partial t} = -\frac{4\kappa L}{r} \to r dr = -4\kappa L dt$$

$$\frac{1}{2}r^2 = -4\kappa L t + B$$

- Since $r(0) = r_0$, then we have $B = \frac{1}{2}r_0^2$,

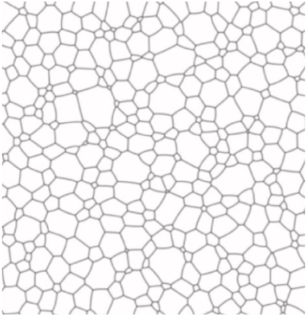
$$r^2 - r_0^2 = -8\kappa L t$$

which is result of sharp interface model.

Multi-order parameter model for grain growth

- How do we extend it to multiple grain cases: Grain 1, Grain 2, $\cdots$, Grain N

$$f(\eta_1, \eta_2, \cdots, \eta_N) = \sum_{i=1}^{N} \left[-\frac{1}{2}\eta_i^2 + \frac{1}{4}\eta_i^4 \right] + \frac{3}{2} \sum_{i=1}^{N} \sum_{j=1}^{j \neq i} \eta_i^2 \eta_j^2$$



Two-grains case

- Assume the presence of η_1 and η_2,

$$f(\eta_1, \eta_2) = -\frac{1}{2}\eta_1^2 + \frac{1}{4}\eta_1^4 - \frac{1}{2}\eta_2^2 + \frac{1}{4}\eta_2^4 + 3\eta_1^2\eta_2^2$$

$$\frac{\partial f}{\partial \eta_1} = -\eta_1 + \eta_1^3 + 6\eta_1\eta_2^2 = \eta_1(-1 + \eta_1^2 + 6\eta_2^2) = 0$$

when $\eta_1 = 1$ and $\eta_2 = 0$.

- N order parameters, N Allen-Cahn equations

$$\frac{\partial \eta_1}{\partial t} = -L\frac{\partial f}{\partial \eta_1}$$

$$\vdots$$

$$\frac{\partial \eta_N}{\partial t} = -L\frac{\partial f}{\partial \eta_N}$$

Profile of two order parameters