Two-Dimensional Dendritic Growth Using Phase-Field Model Mathematical Description

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1 Phenomenon to model

The phenomenon that we model is the phase growth in a bulk of material which has two phases, e.g. the crystalization of water. Mathematical symbols that discribe the system are defined below.

1. $t \in \Re$ is time.
2. $\Omega \subset \Re^N$ is the spatial domain of the system, where N is the spacial dimension of the system.
3. $\boldsymbol{x} \in \Omega$ is the spatial coordinate of the system.
4. $u : (\Omega, \Re) \mapsto \Re$ is a funtion that discribe the dimensionless temperature field.
5. $\phi : (\Omega, \Re) \mapsto [0, 1]$ is a funtion that discribe the phase field. $\phi(\boldsymbol{x}, t) = 0$ means that the material at time t and position $\boldsymbol{x}$ is in phase I; $\phi(\boldsymbol{x}, t) = 1$ means that it is in phas II; $0 < \phi(\boldsymbol{x}, t) < 1$ means it is a mixture of phase I and phase II.
6. C^2 is the function space of any $\phi(\boldsymbol{x})$ that has continuous first 2 derivatives and satisfies required boundary condition.

2 Derivation of the governing equation

In this section, we will derive the governing equation of a specific system. Consider $\Omega = [0, 1] \times [0, 1]$ with periodic boundary condition. The total free energy due to the phase field $\phi(\boldsymbol{x}, t)$ is

$$F = \int f(\phi) + \frac{1}{2} W(\theta(\nabla\phi))^2 |\nabla\phi|^2 d\boldsymbol{x}. \tag{1}$$

In the equation (1),

$$f(\phi) = \frac{\phi^4}{4} - (\frac{1}{2} - \frac{\tilde{n}}{3})\phi^3 + (\frac{1}{4} - \frac{\tilde{n}}{2})\phi^2 \tag{2}$$

is the free energy density of bulk material, where $\tilde{n} = \frac{\beta}{\pi} tan^{-1}[\eta(u_m - u)]$, β and η are material parameters. In the equation (1),

$$W(\theta(\nabla\phi)) = W_0(1 + \mu cos(a_0(\theta - \theta_0)), \tag{3}$$

where $\theta(\nabla\phi)$ is the angle between x-axis and $\nabla\phi$; W_0, a_0 and θ_0 are constants.

We assume that the phase field ϕ changes in the direction in C^2 in which the total free energy F decrease fastest. This means that

$$\tau\frac{\partial\phi}{\partial t} = -\frac{\delta F}{\delta\phi}, \tag{4}$$

where τ is a constant. The functional derivative in the right hand side of equation (4) could be solved by applying the divergence theorem and the periodic boundary condition, which gives

$$\begin{aligned}\tau\frac{\partial\phi}{\partial t} =& \phi(1-\phi)(\phi - \frac{1}{2} + \tilde{n}(u)) - \frac{\partial}{\partial x}(WW'\frac{\partial\phi}{\partial y}) \\ &+ \frac{\partial}{\partial y}(WW'\frac{\partial\phi}{\partial x}) + \nabla(W^2)\cdot\nabla\phi + W^2\nabla^2\phi.\end{aligned} \tag{5}$$

The equation of dimensionless temperature change is

$$\frac{\partial u}{\partial t} = D\nabla^2 u + \frac{1}{2}\frac{\partial\phi}{\partial t}, \tag{6}$$

where D is the thermal diffusion constant and the second term in the right hand side is the latent heat of phase transition.

3 Governing equation in a compact form

In this section, we write all the equations we need in a compact form.

$$\begin{cases}\frac{\partial u}{\partial t} = & D\nabla^2 u + \frac{1}{2}\frac{\partial\phi}{\partial t} \\ \tau\frac{\partial\phi}{\partial t} = & \phi(1-\phi)(\phi - \frac{1}{2} + \tilde{n}(u)) - \frac{\partial}{\partial x}(WW'\frac{\partial\phi}{\partial y}) \\ & + \frac{\partial}{\partial y}(WW'\frac{\partial\phi}{\partial x}) + \nabla(W^2)\cdot\nabla\phi + W^2\nabla^2\phi \\ W = & W_0(1 + \mu cos(a_0(\theta - \theta_0)) \\ \theta = & tan^{-1}(\frac{\partial\phi}{\partial y}/\frac{\partial\phi}{\partial x}) + \pi(1 - sign(\frac{\partial\phi}{\partial x}))\end{cases} \tag{7}$$