

# 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 describe the system are defined below.

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

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

In the equation (1),

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

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

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

where  $\theta(\nabla\phi)$  is the angle between x-axis and  $\nabla\phi$ ;  $W_0, a_0$  and  $\theta_0$  are constants.

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

$$\tau \frac{\partial \phi}{\partial t} = - \frac{\delta F}{\delta \phi}, \quad (4)$$

where  $\tau$  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

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

The equation of dimensionless temperature change is

$$\frac{\partial u}{\partial t} = D \nabla^2 u + L \frac{\partial \phi}{\partial t}, \quad (6)$$

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

### 3 Governing equation in a compact form

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

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