Allen-Cahn equation with anisotropic surface energy

Using ϕ as an order parameter function to define the region of solid: $\phi = 1$ and $\phi = 0$ for solid and liquid regions, respectively. The system's total energy is

$$\mathcal{F} = \int \left(f(\phi) + \frac{1}{2}(\varepsilon \nabla \phi)^2 + ... + h(\phi) m_0(T) \right) d\Omega, \tag{1}$$

where $f(\phi)$ is the bulk free energy of the solid and liquid phases, $(\varepsilon(\theta)\nabla\phi)^2/2$ accounts for the surface energy, $h(\phi)$ is an interpolation function, and $m_0(T)$ is the formation enthalpy. Note that $\varepsilon(\theta)$ is a functional of $\nabla\phi$ since θ is a function of $\nabla\phi$. Some small terms are ignored as "...." in Eq. (1). A mathematically simplified forms of f and h are

$$f(\phi) = \frac{1}{4}\phi^2(1-\phi)^2 \quad \text{and} \quad h(\phi) = \frac{1}{6}\phi^2(3-2\phi). \tag{2}$$

$\mathcal{F}(x, y, \phi, \nabla\phi)$ is a functional of $\phi(x, y)$ and $\nabla\phi(x, y)$ with coordinate variables x and y. The variation of the system energy per ϕ evolution (i.e., the morphology change of the solid) is defined as

$$\frac{\delta \mathcal{F}}{\delta \phi}. \tag{3}$$

Variation derivatives are derivatives of a functional with respect to a function. For Euler-Lagrange equation, if we have

$$J = \int L(x, y(x), y'(x)) dx, \tag{4}$$

then, the variational derivative is

$$\frac{\delta J}{\delta y} = \frac{\partial L}{\partial y} - \frac{d}{dx}\left(\frac{\partial L}{\partial y'}\right). \tag{5}$$

As such, Eq. (3) becomes

$$\frac{\delta \mathcal{F}}{\delta \phi} = \frac{\partial f}{\partial \phi} - \nabla \cdot \left[\frac{\partial}{\partial(\nabla\phi)} \left(\frac{1}{2}\big(\varepsilon(\theta)\nabla\phi\big)^2 \right) \right] + \frac{\partial h}{\partial \phi} m_0(T). \tag{6}$$

For the second term on the RHS, using chain rule for the term in the bracket, we have

$$\nabla \cdot \left[\frac{\partial}{\partial(\nabla\phi)} \left(\frac{1}{2}\big(\varepsilon(\theta)\nabla\phi\big)^2 \right) \right] = \nabla \cdot \left[\varepsilon(\theta)^2 \nabla\phi + \big(\nabla\phi\big)^2 \frac{\partial}{\partial(\nabla\phi)} \left(\frac{1}{2}\varepsilon(\theta)^2 \right) \right]. \tag{7}$$

The term $\partial(\varepsilon^2/2)/\partial(\nabla\phi)$ is a vector field as

$$\left[\frac{\partial}{\partial \phi_{,x}} \left(\frac{1}{2}\varepsilon(\theta)^2 \right), \frac{\partial}{\partial \phi_{,y}} \left(\frac{1}{2}\varepsilon(\theta)^2 \right) \right], \tag{8}$$

where

$$\theta = \tan^{-1}\left(\frac{\phi_{,y}}{\phi_{,x}} \right). \tag{9}$$

Thus,

$$\begin{aligned} \frac{\partial}{\partial \phi_{,x}} \left(\frac{1}{2}\varepsilon(\theta)^2 \right) =& 2 \cdot \frac{1}{2} \cdot \varepsilon(\theta) \frac{\partial \varepsilon(\theta)}{\partial \theta} \frac{\partial \theta}{\partial \phi_{,x}} = \varepsilon\varepsilon' \frac{\partial}{\partial \phi_{,x}} \tan^{-1}\left(\frac{\phi_{,y}}{\phi_{,x}} \right) = \varepsilon\varepsilon' \frac{1}{1 + (\phi_{,y}/\phi_{,x})^2} \frac{\partial}{\partial \phi_{,x}} \left(\frac{\phi_{,y}}{\phi_{,x}} \right) \\ =& \varepsilon\varepsilon' \frac{1}{1 + (\phi_{,y}/\phi_{,x})^2} \cdot \frac{-\phi_{,y}}{(\phi_{,x})^2} = \varepsilon\varepsilon' \frac{-\phi_{,y}}{(\phi_{,y})^2 + (\phi_{,x})^2} = \varepsilon\varepsilon' \frac{-\phi_{,y}}{(\nabla\phi)^2} = -\frac{\varepsilon\varepsilon'}{(\nabla\phi)^2} \cdot \frac{\partial \phi}{\partial y}. \end{aligned} \tag{10}$$

Similarly, for the gradient in the y direction,

$$\begin{aligned} \frac{\partial}{\partial \phi_{,y}} \left(\frac{1}{2}\varepsilon(\theta)^2 \right) =& \varepsilon\varepsilon' \frac{\partial}{\partial \phi_{,y}} \tan^{-1}\left(\frac{\phi_{,y}}{\phi_{,x}} \right) = \varepsilon\varepsilon' \frac{1}{1 + (\phi_{,y}/\phi_{,x})^2} \frac{\partial}{\partial \phi_{,y}} \left(\frac{\phi_{,y}}{\phi_{,x}} \right) \\ =& \varepsilon\varepsilon' \frac{1}{1 + (\phi_{,y}/\phi_{,x})^2} \cdot \frac{1}{\phi_{,x}} = \varepsilon\varepsilon' \frac{\phi_{,x}}{(\phi_{,x})^2 + (\phi_{,y})^2} = \frac{\varepsilon\varepsilon'}{(\nabla\phi)^2} \cdot \left(\frac{\partial \phi}{\partial x} \right). \end{aligned} \tag{11}$$

Substituting Eqs. (10) and (11) into (7), we obtain

$$
\begin{aligned}
&\nabla\cdot\left[\varepsilon(\theta)^2\nabla\phi + \left(\nabla\phi\right)^2\frac{\partial}{\partial(\nabla\phi)}\left(\frac{1}{2}\varepsilon(\theta)^2\right)\right] = \nabla\cdot\varepsilon(\theta)^2\nabla\phi + \nabla\cdot\left(-\frac{\left(\nabla\phi\right)^2}{\left(\nabla\phi\right)^2}\varepsilon\varepsilon'\frac{\partial\phi}{\partial y} + \frac{\left(\nabla\phi\right)^2}{\left(\nabla\phi\right)^2}\varepsilon\varepsilon'\frac{\partial\phi}{\partial x}\right) \\
&\quad = \nabla\cdot\varepsilon(\theta)^2\nabla\phi - \frac{\partial}{\partial x}\left(\varepsilon\varepsilon'\frac{\partial\phi}{\partial y}\right) + \frac{\partial}{\partial y}\left(\varepsilon\varepsilon'\frac{\partial\phi}{\partial x}\right) = \nabla\cdot\varepsilon(\theta)^2\nabla\phi - \frac{\partial\varepsilon\varepsilon'}{\partial x}\cdot\frac{\partial\phi}{\partial y} - \varepsilon\varepsilon'\frac{\partial^2\phi}{\partial x\partial y} + \frac{\partial\varepsilon\varepsilon'}{\partial y}\cdot\frac{\partial\phi}{\partial x} + \varepsilon\varepsilon'\frac{\partial^2\phi}{\partial y\partial x} \\
&\quad = \nabla\cdot\varepsilon(\theta)^2\nabla\phi - \frac{\partial\varepsilon\varepsilon'}{\partial x}\cdot\frac{\partial\phi}{\partial y} + \frac{\partial\varepsilon\varepsilon'}{\partial y}\cdot\frac{\partial\phi}{\partial x}.
\end{aligned} \tag{12}
$$

Putting everything together, Eq. (6) becomes

$$
\frac{\delta\mathcal{F}}{\delta\phi} = \left(\frac{1}{2}\phi(1-\phi)(1-2\phi)\right) - \left(\nabla\cdot\varepsilon(\theta)^2\nabla\phi - \frac{\partial\varepsilon\varepsilon'}{\partial x}\cdot\frac{\partial\phi}{\partial y} + \frac{\partial\varepsilon\varepsilon'}{\partial y}\cdot\frac{\partial\phi}{\partial x}\right) + \phi(1-\phi)m_0(T), \tag{13}
$$

where

$$
m_0(T) = \frac{\alpha}{\pi}\tan^{-1}\left(\gamma(T-T_m)\right). \tag{14}
$$