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Competing effects of interface anisotropy and isotropic driving force on the growth of steady-state shape in phase-field modeling

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ABSTRACT

It is well-known that the Wulff construction represents the steady-state shape during a shrink evolution in the anisotropic Allen–Cahn phase-field model (AC-PFM). Adding a constant driving force (ΔF_{mc}) into the AC-PFM will result in the competition between the anisotropic shrink and the isotropic growth, which may lead to different phase shape at the steady state. Through numerical simulations and theoretical analyses, three types of evolution behaviors that depend on the strength of ΔF_{mc} have been concluded: shrink resembling Wulff, growth resembling Wulff and growth deviating from Wulff. In other words, in the limit of $\Delta F_{mc} \to 0$, the steady-state shape predicted by PFM follows the Wulff shape, but deviates from Wulff when ΔF_{mc} grows substantially, as the ΔF_{mc} term represents the isotropic feature of the growth dynamics while the other parts denote the anisotropic feature in the Wulff shape. The equivalence of the steady-state shape to Wulff when $\Delta F_{mc} \to 0$ has been proven based on a numerically verified interface normal velocity model. The "critical" ΔF_{mc} for marked deviation from Wulff estimated from order analysis of the system evolution equation, is very closed to the point where the normal velocity (V_n) changes its dependence on ΔF_{mc} from $V_n \propto \Delta F_{mc}$ to $V_n \propto (\Delta F_{mc})^{0.5}$.

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1. Introduction

Many thermodynamic and kinetic parameters of materials are anisotropic, such as elastic constants, diffusion coefficients, and surface/interfacial energies. These anisotropies have great effects on the evolution dynamics and/or the final microstructural morphology in materials processing. Particularly, anisotropy of interfacial energy is considered to be responsible, at least partially, for some special morphology of the new phases in phase transition, such as dendrite in solidification [1–3] and Widmanstätten microstructure in austenite–ferrite transformation [4–6].

Phase-field modeling (PFM), in which interfacial anisotropy can be conveniently considered, has been proven to be a powerful tool for microstructure evolution simulation [7–9]. In PFM, the free energy density for a structurally non-uniform system is comprised of chemical free energy and interfacial energy in a form typically like $f(\phi, \nabla\phi) = f_0(\phi) + \frac{\varepsilon^2}{2}|\nabla\phi|^2$, where f_0 is the chemical free energy density, ϕ is the phase-field order parameter and ε is the gradient energy coefficient. The interfacial anisotropy can be introduced by making ε orientation-dependent. For example a general form, $\varepsilon = \varepsilon_0[1 + \gamma\cos(k\theta)]$, is proposed for two-dimensional simulations [10], where ε_0 is the mean value, θ is the angle between the unit normal vector of the interface and a reference direction, γ is the amplitude of anisotropy and k is the folds of symmetry. Based on this general form, many variants have been adopted for different applications [4,11]. For three-dimensional problems a form, $\varepsilon = \varepsilon_0[1 + \gamma(n_x^4 + n_y^4 + n_z^4)]$, is made by Karma and Rappel [2] for cubic metals, where n_x, n_y and n_z are Cartesian coordinates of the interface normal vector $\hat{n}$. More recently, another form $\varepsilon = \varepsilon_0 + \varepsilon_1(n_x^2n_y^2 + n_y^2n_z^2 + n_z^2n_x^2) + \varepsilon_2 n_x^2n_y^2n_z^2 + \varepsilon_3(n_x^2n_y^2 + n_y^2n_z^2 + n_z^2n_x^2)^2$ is suggested by Qin and Bhadeshia [12] with more terms for wider representation, where ε_1, ε_2 and ε_3 are anisotropy coefficients which can be determined experimentally or assessed using computational methods. The "interface" in this study could be either amorphous–crystal or crystal–crystal interface. In the latter case, note that generally the interfacial energy depends on both the interface orientation and the misorientation of the crystals across

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the interface, just like the five freedoms a grain boundary has. However once the misorientation of the neighboring crystals across the interface is fixed, the interfacial energy varies only with respect to the orientation of the interface; that is the case represented by the above form by Qin and Bhadeshia [12].

The characteristics of dynamics of systems with interfacial anisotropy in PFM models have been extensively investigated, especially the shape evolution of particles embedded in a matrix phase. For conserved systems described by the Cahn–Hilliard (CH) equation [13,14], the equilibrium shape is found to be identical with the prediction from Wulff's theorem that gives the minimum total surface/interface energy for a volume-fixed particle with anisotropic surface/interface energies [15,16]. For non-conserved systems described by Allen–Cahn (AC) equation [17,18], there is no equilibrium state; instead a steady-state shape, in other words, a self-similar shape, can be obtained. Driven by the curvature effect alone, the particles will shrink and evolve into a steady-state shape that is identical with what predicted by the Wulff's theorem, which has been analytically proved by Taylor and Cahn [19] and others [20,21]. Moreover, people studied the situation when the AC model is supplemented with a constant-volume constraint reserving the volume of the product phase, and found that the final stationary state is still consistent with the Wulff shape [22].

A typical Allen–Cahn model as above mentioned only considers the curvature effect, and it is very common to introduce other additional physical driving forces [12,23]. A simple example would be adding a constant isotropic phase transformation driving force, e.g., the system is chemically uniform and consequently there is no diffusion involved. Under such circumstance, the steady-state shape could be markedly deviated from the Wulff shape [12]. Here we propose a hypothesis trying to explain this deviation of the steady-state shape from the Wulff shape. We postulate that the additional phase transformation driving force should contribute to the particle's steady-state shape, i.e., there exists a competition of the isotropic driving force with respect to the anisotropic curvature effect. However, to our best knowledge, this hypothesis, including the relative strength of the competition and its detailed effects for the similarity between the two shapes, has not been testified yet. Therefore, the motivation for the present work is to systematically analyze the above competing effects, more specifically, to evaluate their influence on the similarity between the PFM and Wulff predictions, and to locate possible transition points between different morphological features and so on.

Correspondingly this paper is organized as follows. We first briefly summarize the theory of non-conserved PFM with interfacial anisotropy, and the overall features of the morphology evolution of the product phase are analyzed based on the master equation for the evolution of the system in Section 2. Numerical simulation results are presented in Section 3 to give a quantitative evaluation of the competition effects of the interfacial anisotropy and the phase transformation driving force. Finally, steady-state shapes are classified according to their similarities to the Wulff shape, and theoretical illustrations for typical evolution features are discussed.

2. Phase field method

Phase-field modeling (PFM) is a powerful framework to incorporate various physical energies/effects in the simulation of microstructural evolution in phase transformations. The fundamental idea is to use continuum field variables ϕ to denote the phases in the system; and the evolution of the microstructure is represented by the temporal evolution of the field variables ϕ driven by the reduction in the free energy of the system. The significant computational advantage is that it avoids explicit tracking and setting up rules of evolution for the interfaces. For a system with a single phase variable, the total free energy is given by an integral of the free energy density over the total volume:

$$F = \int_{\Omega} \left(f_0(\phi) + \frac{\varepsilon^2}{2} |\nabla \phi|^2 \right) dV \tag{1}$$

where the chemical free energy density f_0 is chosen in a double-well function form [24,25]:

$$f_0(\phi) = [1 - h(\phi)] f_m + h(\phi) f_c + \frac{1}{4w} g(\phi) \tag{2}$$

where f_m and f_c are the free energy density of the two bulk phases, the matrix phase denoted by $\phi = 0$ and the child phase by $\phi = 1$, respectively; a non-zero difference in f_m and f_c ($\Delta F_{mc} = f_m - f_c > 0$) constitutes a constant driving force for phase transformation. $h(\phi)$ is the interpolation function that should satisfy the following requirements: it is a monotonic function in [0, 1] with $h(0) = 0$ and $h(1) = 1$; and the chemical free energy density should have two minima in the two bulk phases as $\left.\frac{\partial h(\phi)}{\partial \phi}\right|_{\phi=0,1} = 0$. $g(\phi) = \phi^2(1-\phi)^2$ is the double-well potential function, which guarantees the free energy density has two local minima at $\phi = 0$ and $\phi = 1$. The energy barrier parameter w is a coefficient reflecting the kinetic barrier between the two minima. The coefficients w and ε are analytically related to two physical quantities, the interfacial energy $\sigma = \varepsilon/(6\sqrt{2w})$ and the interface thickness $2\lambda = 4.2\varepsilon\sqrt{2w}$ [12]. The temporal evolution of $\phi(\vec{r}, t)$ ($\vec{r}$ denotes the location of the material point) follows the Allen–Cahn equation [17,18]:

$$\frac{\partial \phi}{\partial t} = -M_\phi \frac{\delta F}{\delta \phi} \tag{3}$$

where M_ϕ is the kinetic coefficient characterizing the interface mobility and can be derived from the interface kinetics [26–29] and $\delta F/\delta\phi$ is the functional derivative of the free energy functional with respect to the phase-field variable.

Now we introduce the desired orientational anisotropy into PFM by making ε varies as a function of the interface normal vector $\hat{n}$:

$$\hat{n} = \frac{\nabla \phi}{|\nabla \phi|} \tag{4}$$

This gives $n_i = \phi_{,i} \Big/ \sqrt{\sum_i \phi_{,i}^2}$, where i represents one of the axes in Cartesian coordinates and $\phi_{,i} = \partial\phi/\partial x_i$. The gradient energy coefficient can be represented as $\varepsilon(\hat{n}) = \varepsilon_0 \eta(\hat{n})$, where $\eta(\hat{n})$ is the anisotropy function and expressed as [12]:

$$\eta(\hat{n}) = 1 + \frac{\varepsilon_1}{\varepsilon_0}(n_x^2 n_y^2 + n_y^2 n_z^2 + n_z^2 n_x^2) + \frac{\varepsilon_2}{\varepsilon_0} n_x^2 n_y^2 n_z^2 + \frac{\varepsilon_3}{\varepsilon_0}(n_x^2 n_y^2 + n_y^2 n_z^2 + n_z^2 n_x^2)^2 \tag{5}$$

Three typical sets of parameters are listed in Table 1 and the corresponding polar diagrams are presented in Fig. 1. These values are used in the following numerical simulations, and are chosen to be identical to those adopted in Ref. [12] for the sake of comparison.

Strong anisotropy leads to artificial "ears" in the Wulff shapes as for cases A and C if the Wulff shape is constructed by the paramet-

Table 1
Coefficients of the anisotropy function applied in phase-field models.

	Case A	Case B	Case C
$\varepsilon_1/\varepsilon_0$	−0.863	0.402	1.8655
$\varepsilon_2/\varepsilon_0$	0.395	0.00144	0.2555
$\varepsilon_3/\varepsilon_0$	0.0238	0.00066	0

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