Current development in quantitative phase-field modeling of solidification

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ARTICLE INFO	ABSTRACT
	The quantitative phase-field simulations were reviewed on the processes of solidification of pure metals and alloys. The quantitative phase-field equations were treated in a diffuse thin-interface limit, which enabled the quantitative links between interface dynamics and model parameters in the quasi-equilibrium simulations. As a result, the quantitative modeling is more effective in dealing with microstructural pattern formation in the large scale simulations without any spurious kinetic effects. The development of the quantitative phase-field models in modeling the formation of microstructures such as dendritic structures, eutectic lamellas, seaweed morphologies, and grain boundaries in different solidified conditions was also reviewed with the purpose of guiding to find the new prospect of applications in the quantitative phase-field simulations.

1. Introduction

The formation of microstructures during solidification has fascinated researchers in materials science, materials physics and many other fields for decades of years[1-6]. Understanding of solidification microstructures underlies various issues of scientific and industrial importance to study material properties of alloys castings[7], for instance, the dendritic and cell growth with the phase transition, competition between oriented grains, domain formation for microstructural defects, etc. Therefore, it is crucial to control and predict microstructure formation during different solidification processes. Recent progresses in experimental techniques have improved the understanding of intriguing phenomena and mechanisms of microstructural formation. In particular, the development of synchrotron X-ray imaging techniques[8-14] has enabled the in situ observation of metallic material solidification. However, the real-time investigations of microstructure formation and the associated segregation patterns are still lacking[7]. Furthermore, those in situ observa-

tions are only restricted in the thin samples that are essentially quasi-two-dimensional involving only a finite number of alloy systems, whereas the collective behavior of various complex alloy systems in three-dimensional system is of primary importance in controlling the solidification microstructures.

Numerical simulations are regarded as the promising methods to better understand alloy microstructural formation in a systematic, efficient and cost effective manner[7]. For instance, molecular dynamics (MD)[15-18] and Monte Carlo (MC)[19-21] simulations are of great value in understanding the microscopic formation of solidification patterns, especially in the study of nonequilibrium growth dynamics in related to the microstructure instability. The dynamic mean-field approach[22-24] is effective to study the competitive mechanism between nucleation and grain growth. However, these methods are difficult to deal with the interfacial evolution in a complex boundary problem, which is very common in solidification of alloys.

The phase-field method has emerged as an effective tool in modeling complex microstructures for

solidification transformations. It is based on the Ginzberg-Landau theory of phase transitions with minimizing a thermodynamically consistent free energy functional in terms of field variables. In phase-field models, the liquid-solid interface is extended into a virtual diffuse interface, where states are quantified by a spatially distributed order parameter, i. e., phase field. Since one does not need to explicitly track boundary motions with complex patterns, the phase-field method has been commonly used in solidification of pure materials as well as binary, multicomponent and multi-phase alloys with a variety of microstructural pattern formations[25-28]. Furthermore, phase-field models have attracted a significant number of attentions with great research interests in many other growth dynamic processes with different scales, such as epitaxial film growth[29-33], domain evolution in ferromagnetic and ferroelectric materials[34-37], electrochemical reaction[38-42], and the evolution of nerve cells[43,44], owing to their fundamental nature in related to phase transformations.

However, it should be noted that solidification has a multi-scale nature in physics. The length scales span from several nanometers thicknesses for liquid-solid interfaces to tens or hundreds of microns for microstructural morphologies; the time scales span from picoseconds for atomic attachment to seconds for heat or solute diffusion[7]. It remains difficult to capture microstructural evolution over such multiple length and time scales using phase field and many other numerical simulations, which presents as a great challenge in the modeling of solidification.

In recent years, a series of new phase-field models have been developed in solidifications, which enables more quantitative descriptions in the diffuse thin-interface limit[45], where the scale of interface thickness is considerably larger than the capillary length. Quantitative phase-field models have an advantage in establishing relationships of the characteristics of interface dynamics with the model parameters in the steady state simulations. Furthermore, the quantitative modeling is able to eliminate the spurious kinetic effects arising from the large values of interface thicknesses. For instance, an anti-trapping current[45,46] is proposed to adjust the solute distribution and avoid the abnormal solute trapping. This allows quantitative comparisons between experiments and predictions of microstructural pattern formation for the considerably large scale simulations both in two and three dimensions.

2. Principle of Quantitative Phase-field Model

The first fully quantitative model was proposed by Karma and Rappel[47-49]. They reported dendritic growth with pure undercooled melt using a quanti-

tative phase-field method. Considering a simplest dendrite growth model in solidification of a pure material, the sharp interface model can be described by the following equations,

$$\partial_t u = D \nabla^2 u \tag{1}$$

$$v_n = D(\partial_n u^- - \partial_n u^+) \tag{2}$$

$$u_i = -d_0 \kappa - \beta v_n \tag{3}$$

where, $u = (T - T_M)/(L/C_p)$ is denoted by the dimensionless temperature field; t is the time; T is the environmental temperature; T_M is the melting temperature; L is the latent heat of melting; and C_p is the specific heat at constant pressure. Far from the interface, $u = -\Delta$, where $\Delta = (T_M - T_\infty)/(L/C_p)$ is the dimensionless undercooling and T_∞ is the initial temperature of the undercooled liquid. D is the diffusion coefficient; v_n is the normal interface velocity with the unit vector $\boldsymbol{n}$ pointing to the normal interface direction, and $\partial_n u^-$ and $\partial_n u^+$ denote the normal derivative of u on the liquid ($+$) and solid ($-$) sides of the interface, respectively. Eq. (3) is a velocity-dependent form of the Gibbs-Thomson condition, which incorporates the nonequilibrium kinetics of the interface. d_0 is the capillary length; κ is the local principal curvature of the interface, and β is the interface kinetic coefficient. Note that both d_0 and β are related to the surface energy anisotropy, i. e., $d_0 \equiv d_0(\boldsymbol{n})$ and $\beta \equiv \beta(\boldsymbol{n})$. In three dimensions, the curvature term can be extended into a more common form,

$$d_0 \kappa \equiv \sum_i^2 \left[\gamma(\boldsymbol{n}) + \frac{\partial^2 \gamma(\boldsymbol{n})}{\partial \theta_i^2} \right] \kappa_i \tag{4}$$

where, $\gamma(\boldsymbol{n}) = \gamma_0 a_s(\boldsymbol{n})$ is the anisotropic surface energy; γ_0 is the isotropic part of surface energy; $a_s(\boldsymbol{n})$ measures the spatially distributed shape of anisotropy; and κ_i is the local principal curvatures of the interface. Here, $\boldsymbol{n}$ is the unit vector normal to the interface and θ_i are the angles between the normal $\boldsymbol{n}$ and the two local principal directions on the boundary. The anisotropic phase-field model can be described by

$$F = \int [W^2(\boldsymbol{n}) |\nabla \phi|^2 + f(\phi) + \lambda u g(\phi)] dr \tag{5}$$

$$\tau(\boldsymbol{n}) \partial_t \phi = -\frac{\delta F}{\delta \phi} \tag{6}$$

$$\partial_t u = D \nabla^2 u + \frac{1}{2} \partial_t h(\phi) \tag{7}$$

where, $\boldsymbol{r} = (x, y, z)$ denotes the spatial position; F is the free energy functional; W and τ are the anisotropic spatial and time parameters, isotropic parts of which (denoted by W_0 and τ_0) evaluate the characteristic length and time scale, respectively; $f(\phi)$ is a double well potential function, with minima at $\phi = -1$ and $\phi = +1$ that correspond to the liquid and solid phases, respectively; $g(\phi)$ is introduced to link the minima of the free energy with the diffusion field; λ is a dimensionless coupling coefficient; $h(\phi) = \phi$ is the simplest function which incorporates latent heat