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Phase field modeling with large interface thickness and undercooling

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ABSTRACT

The interface thickness is the most crucial parameter in the phase field model (PFM) for the accuracy and the computability. However, the Gibbs–Thomson equation can be satisfied only when the interface thickness is sufficiently small, especially with a large undercooling, but this greatly limits the applications of PFM to a realistic problem. The temperature correction in the thin-interface model partially resolves the problem, but the range is rather limited. In this report, we propose a new formulation of PFM by adding extra terms stabilizing the hyperbolic tangent profile of the phase-field, and this allows us to use a much larger interface thickness for simulation, even with a large undercooling. Several benchmark comparisons with analytical solutions are carried out and discussed.

1. Introduction

The phase-field model (PFM) has emerged as a powerful tool for the simulation of solidification and crystal growth, especially involving microstructure development [1–4]. In contrast to the front tacking method, the phase-field model introduces a continuous phase-field variable ϕ to describe the interface through a rapid transition function. However, the diffusive interface does not represent the sharp interface limit unless the interface diffusion length W is near the capillary length d_o, i.e, the coupling constant $\lambda=a_1W/d_0$ being in the order of unity; a_1 is a positive constant of order unity [1]. This makes the simulation of a realistic physical problem using PFM very difficult from the computational point of view. The thin-interface model developed by Karma and Rappel [5,6], greatly relaxes this requirement and allows the interface thickness to be the suborder of the radius of curvature of the interface, i.e, the tip radius in dendritic growth. Their works provide a relation between the parameters of the original sharp-interface model and the PFM, and have been the starting point for the quantitative computations of solidification in the regime, where the capillary effect dominates the interface kinetics [7]. Nevertheless, λ still cannot be too large.

We have examined the limitation of λ and found that λ is restricted by $\lambda\Delta_i<1$, where $\Delta_i=(T_m-T_i)/(\Delta H/C_p)$ is the undercooling at the interface; ΔH and C_p are the heat of fusion and the heat capacity. This restriction cannot be relaxed by just predicting the correct interface temperature as in the thin-interface model. Similar observation has also been reported by others [8–10] that the phase field should remain sufficiently close to its equilibrium profile for the perturbative expansion to remain valid, i.e., the dimensionless interface velocity $V^*<1$. In other words, the relaxation time in the phase-field equation needs to be smaller than the time for the interface to move across its thickness. To further relax the restriction of λ and interface undercooling, Bragard et al. [10] used the effective function $h(\lambda\Delta_i)$ instead of $\lambda\Delta_i$ to simulate Nickel dendrites that additional calculations of h and Δ_i are needed. Miller et al. [11–12] used two different kinds of interface thicknesses; however, their model is complicate and difficult to implement for computation.

In this paper, we discuss the source of errors for large λ and then propose a new formulation of the thin-interface PFM by adding extra terms stabilizing the hyperbolic tangent profile of the phase-field. With this new formation, a much larger λ can be used and some benchmark comparisons with analytical solutions are given and discussed. In the next session, we begin with the introduction of the sharp- and thin-interface modes. Then, we describe how we come to the new formation. Some results and discussion are given in Section 3 before the conclusion in Section 4.

2. Phase field models

2.1. The sharp-interface model

The simplest phase field equation having an isotropic interfacial energy [13] can be written as

$$\tau\frac{\partial\phi}{\partial t}=W^2\nabla^2\phi-f_\phi(\phi)-\lambda T^*g_\phi(\phi), \tag{1}$$

where τ is the characteristic time and ϕ the phase field variable ranging from −1 (melt) to 1 (solid); ϕ is set to zero at the interface

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and $T^*=(T-T_m)/(\Delta H/C_p)$ the dimensionless temperature. The function $f(\phi)+\lambda T^* g(\phi)$ is a phenomenological free energy, where $f(\phi)$ is a double well potential and $g(\phi)$ shifts the relative height of the two minima of the function making one of the phases metastable for $T^*\neq 0$. The simplest choice of $f(\phi)$ that has been widely used is

$$f(\phi)=-\frac{\phi^2}{2}+\frac{\phi^4}{4}. \tag{2}$$

The advantage of using this function is that ϕ can has the asymptotic solution of

$$\phi=\tanh\left(\frac{x_n}{\sqrt{2}W}\right) \tag{3}$$

for small λT^*, where x_n is the normal distance from the interface with the direction from the liquid to solid sides [6]. Different choices of $g(\phi)$ can result in different phase field models. For the minima of free energy at $\phi=\pm 1$ independent of T^*, $g(\phi)$ can be chosen as [6]

$$g(\phi)=\varphi-\frac{2\phi^3}{3}+\frac{\phi^5}{5}. \tag{4}$$

The above PFM is developed to describe the Gibbs–Thomson (GT) equation at the solidification interface, i.e.,

$$\beta V=-d_0\kappa-T_i^*, \tag{5}$$

where β is the kinetic coefficient, V the interface velocity, and κ the interface curvature; the subscript i indicates the interface. The phase-field model and the GT equation can then be connected by the relationship of (τ, W, λ) and (d_o, β) [4,13] as the following:

$$W=\lambda d_0/a_1, \tag{6}$$

$$\tau=\lambda W\beta/a_1, \tag{7}$$

where the constant a_1 depends on the choice of $g(\phi)$ [14]. Again, λ or W needs to be small enough in the model to satisfy the GT equation. In other words, T^* at the interface calculated from the PFM can converge to T_i^* only when λ or W is small enough, i.e., in the order of the capillary length d_0. This is the so-called sharp-interface limit [15,16].

2.2. The thin-interface model

The thin-interface model [6] extends the interface thickness W to the sub-order of the radius of the curvature of the interface, but the original characteristic time should be replaced by

$$\tau_{thin}=\lambda W\beta/a_1+a_2\lambda W^2/D, \tag{8}$$

where a_2 is a constant and D thermal diffusivity. The thin-interface model is very powerful, and greatly reduces the computational effort. With this model, adaptive mesh refinement is further used to simulate quantitatively the dendritic growth at low undercooling in two-dimensional [17] and three-dimensional [18].

The above thin-interface model is accurate for the simulation in the regime that is dominated by the capillary effect. On the other hand, for the regime dominated by the interface kinetics, such as the faceted growth of silicon, Vetsigian et al. [19] further modified the model by adding a correction term, as a function of ϕ and the Peclet number to extend the available range of λ. With this modification, the sharp-interface temperature is described more accurately through the diffusion behavior of temperature in the diffusive interface.

An interesting observation is that the above models by finding the right interface temperature should be the same as the sharp-interface model if the temperature is uniform or the thermal diffusivity is infinite. This could be demonstrated by a simple 1D solidification problem with a uniform undercooling Δ, where growth rate is Δ/β from Eq. (5). Because the interface temperature is the same, the PFM is the same for both sharp and thin interfaces. The dimensionless growth speed should be the same and be the function of $\lambda\Delta$ only. When λ is small enough, V would converge to Δ/β or V^* to $\lambda\Delta/a_1$, where $V^*=V\tau/W$. Also, since different choices of the characteristic time, the growth velocity can further be rewritten as follows:

$$V_{sharp}=V^*W/\tau=\Delta/\beta,, \tag{9}$$

$$V_{thin}=V^*W/\tau_{thin}=\Delta/\beta/(1+a_2\lambda d_0/D\beta). \tag{10}$$

Because the growth velocity in Eqs. (9) and (10) should be the same, the thermal diffusivity should be set to infinite in Eq. (10) for uniform temperature. Otherwise, the growth velocity is a function of $d_0/D\beta$; however, the correct growth velocity is a constant (Δ/β). This seems to be an interesting starting point for the discussion of the convergence of the PFM to the GT equation.

2.3. The new formation

As just mentioned, we observed that as λ is increased, the simulated phase field variable departs from the hyperbolic tangent (tanh) distribution, i.e., Eq. (3). For an accurate computation, λ is restricted by $\lambda\Delta_i<1$ or $V^*<1$, and this cannot be corrected by just finding the correct interface temperature.

To test the limit of λ, we consider a 1D problem with a given temperature profile first. For a linear temperature profile $T^*=Gx/W$, the calculated phase field variable distributions are shown in Fig. 1 for different λG values; G is the dimensionless temperature gradient. As shown, the calculated phase field variable departs from the tanh distribution with the increasing λG; here $\lambda G=0.1\sim16$. As will be discussed shortly, as the phase field departs from the tanh distribution, the error in the GT equation increases as well. To explain the diffusion behavior of ϕ from the tanh distribution and its effect on the error in the GT equation, we examine the PFM from based on the geometric derivation proposed by Beckermann et al. [20] as follows.

For a 2D problem with an isotropic interfacial energy, the GT equation (Eq. (5)) could be rewritten using the phase field variable as

$$\beta\frac{\partial\phi/\partial t}{\partial\phi/\partial x_n}=d_0\frac{\partial^2\phi/\partial {y_n}^2}{\partial\phi/\partial x_n}-T_i^*, \tag{11}$$

where x_n and y_n are the coordinates defined by the normal and tangential directions of the interface. For 3D problems, $\partial^2\phi/\partial {y_n}^2$ can also be replaced by $\nabla^2\phi-\partial^2\phi/\partial {x_n}^2$.

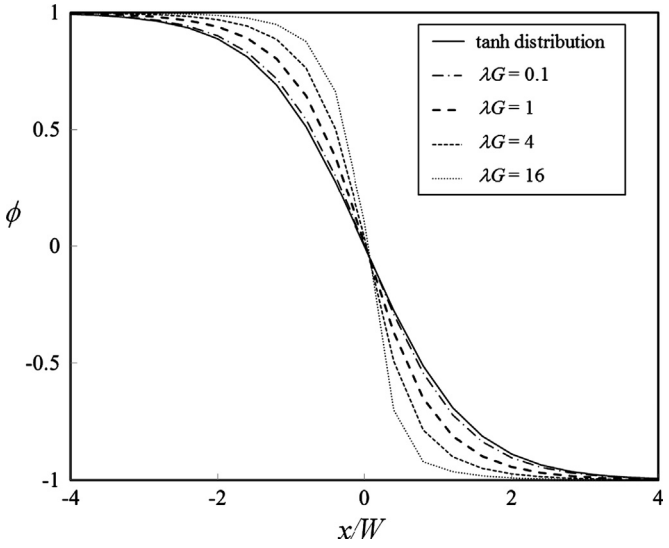

Fig. 1. Phase distribution with different λG values and the comparison with the exact tanh distribution, where $\lambda G=0.1\sim16$.