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Numerical testing of quantitative phase-field models with different polynomials for isothermal solidification in binary alloys

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ABSTRACT

Quantitative phase-field models have been developed as feasible computational tools for solving the free-boundary problem in solidification processes. These models are constructed with some polynomials of the phase-field variable that describe variations of the physical quantities inside the diffuse interface. The accuracy of the simulation depends on the choice of the polynomials and such dependence is indispensable for high-performance computing and valuable for extending the range of applications of the model to several physical systems. However, little is known about the dependence of the accuracy on the choice of the polynomials. In this study, numerical testing is carried out for quantitative phase-field models with extensive sets of polynomials (24 different models) for isothermal solidification in binary alloys. It is demonstrated in two-dimensional simulations of dendritic growth that a specific set of polynomials must be employed to achieve high accuracy in the models with double-well and double-obstacle potentials. Both types of model with the best set of polynomials yield almost the same numerical accuracy.

1. Introduction

Accurate control of the solidification microstructures in alloys is an issue of great importance in the field of metallurgy because microstructural features such as the size and morphology of the solidified grains and microsegregation directly determine the properties of the as-cast alloys. Several methods have been developed for simulation of solidification microstructures on the basis of the sharp-interface description [1–4] and also the diffuse-interface description. The phase-field model is a diffuse-interface model for describing microstructural processes in solidification [5–9]. It serves as a viable computational tool for solving the free-boundary problem (FBP) of solid–liquid interfaces. Although phase-field model generally has a high computational cost, recent advances in parallel computing techniques have enabled large-scale phase-field simulations of the competitive growth of a bunch of dendrites [9,10]. Furthermore, progress has been made in evaluating the input parameters in the phase-field model on the basis of atomistic simulations [10–12]. Such progress has rapidly increased the effectiveness of phase-field simulations for analyzing and controlling solidification microstructures.

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In the phase-field model, the interface is not sharp but a diffuse entity having a thickness. Since state variables such as the order parameter called the phase-field variable and the concentration field(s) change continuously inside the interface, the computational cost increases with decreasing interface thickness. The interface thickness must be chosen to be much larger than the atomic distance but smaller than any length scale relevant to the microstructure (e.g., the tip radius of a dendrite). Therefore, the interface thickness in this model is a constant determined by the scale of microstructure and the computational cost. When a finite value is assigned to the thickness, however, it is difficult to use early models in a quantitative manner. The early models are called standard phase-field models in this paper. This problem arises because the standard models were constructed to reproduce the solution of the FBP in the limit of zero thickness (the sharp-interface limit). In an actual simulation with a finite thickness, they suffer from unphysical magnification of the interface effects, causing an undesired dependence of the simulation result on the thickness. This serious problem was resolved in so-called quantitative phase-field models [13–21]. These quantitative models were constructed on the basis of the thin-interface asymptotics, where the model is mapped onto the FBP in the limit of non-zero thickness. The first quantitative model was proposed for solidification in a pure substance with symmetric diffusion (i.e., equal thermal diffusivity in the liquid and solid phases) [13], and it was extended to deal with alloy solidification with one-sided diffusion [13–18] (negligible solute diffusivity in the solid) and also two-sided asymmetric diffusion (non-zero solute diffusivity in the solid) [19–21]. The essential ingredient in the quantitative phase-field models for alloy systems is the so-called anti-trapping current, a correction term for the diffusion flux inside the interface [14]. Although this correction term was introduced in a phenomenological manner in the early models, variational formulations of quantitative phase-field models including the anti-trapping current have recently been demonstrated for a pure substance [22] and for a binary alloy system with two-sided asymmetric diffusion [23].

Quantitative phase-field models were developed as an effective alternative to the FBP and have been increasingly utilized to simulate solidification microstructures [24–32]. It is important to point out that there are several possible forms of quantitative phase-field models and that not all the models yield accurate numerical solutions. In the phase-field models, continuous variations of the physical quantities inside the interface are described by polynomials of the phase-field variable, which are called interpolating functions in this paper. As demonstrated in an early study [13], different forms of the interpolating function related to the enthalpy result in different numerical accuracy for dendritic growth in a pure substance. In the case of isothermal solidification in a binary alloy, which is our main concern, four types of interpolating function must be introduced to represent the continuous variations of the barrier potential between the solid and liquid, the bulk's free energy densities (driving force), the concentration field and the diffusivities. There are various possible forms for each interpolating function and a different set of functions should result in different numerical accuracy. However, little has been clarified regarding the accuracy of models with different sets of interpolating functions. For instance, either the double-well potential [13–29] or the double-obstacle potential [30–36] has been employed to represent the barrier potential in the standard and quantitative phase-field models. Each potential offers different advantages in terms of ease of implementation, applicability to multiphase systems and so forth. However, it is not clear which potential is superior in terms of numerical accuracy because a fair comparison between them has not been carried out in the framework of quantitative simulations. Note that only a few sets of interpolating functions have so far been employed in quantitative phase-field simulations [13–32]. Models with the other sets of functions have not yet been implemented and hence they have not been subjected to numerical testing. The dependence of the numerical accuracy on the choice of interpolating functions is important information in the development of quantitative phase-field models for a variety of physical systems. In addition, finding the best set of interpolating functions is an issue of great interest in the high-performance computing of solidification microstructures.

The main purpose of this study is to elucidate the dependence of the numerical accuracy of quantitative phase-field models on the choice of the interpolating functions and also to find the best set of functions by performing detailed comparisons of the numerical accuracy between them. The numerical testing is carried out for 24 different quantitative models. It is found that models constructed with the double-well and double-obstacle potentials yield comparably good numerical accuracy as long as the best set of interpolating functions is employed. In the next section, we provide a brief explanation of the quantitative phase-field models and interpolating functions. Detailed comparisons of the accuracy between the models are demonstrated by performing one-dimensional simulations of a moving flat interface and two-dimensional simulations of dendritic growth in Sec. 3. The conclusions are given in Sec. 4.

2. Quantitative phase-field models and computational details

2.1. Model for isothermal solidification in a dilute binary alloy

In this study, we focus on isothermal solidification in a dilute binary alloy which is a simple case suitable for the present purpose. We consider a dilute alloy with a constant partition coefficient k, constant diffusivity in the liquid D_l and negligible solid diffusivity (i.e., one-sided diffusion). Then, the sharp-interface equations for the moving solid–liquid interface are given as

$$\partial_t c_l = D_l \nabla^2 c_l, \tag{1}$$

$$(1-k) c_l V_n = -D_l \partial_\eta c_l|^*, \tag{2}$$

$$\frac{c_l^*}{c_l^e} = 1 - (1-k) d_0 K - (1-k)\beta V_n, \tag{3}$$