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Phase-field simulation during directional solidification of a binary alloy using adaptive finite element method

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Abstract

We have performed phase-field simulations during directional solidification of a binary alloy. Adaptive mesh refinement techniques, in which the degrees of freedom of additional hanging nodes which occur when a quadrilateral element is refined are eliminated by matrix operations, are introduced to the finite element analysis in order to conduct the phase-field simulations efficiently. The validity of the numerical techniques presented here is ascertained by comparing the numerical results of the absolute stability limit and the onset of instability with those calculated from the Mullins–Sekerka theory and from the good linear relationship between $\log(V)$ and $\log(\lambda)$, in which the simulations under the constant concentration and temperature gradient are conducted by varying the pulling velocity. Furthermore, we examine the morphology change from cellular to dendritic structure and the relationship between $\log(\lambda)$ and $\log(G)$ for varying the temperature gradient.

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1. Introduction

In the directional solidification of binary alloy systems, the morphological transition from the planar interface to the periodic dendritic or cellular structure is a phenomenon attracting much interest and an important problem. Therefore, experimental, theoretical, and numerical studies on directional solidification

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have been carried out over the past 50 years [1]. Above all, due to the rapid progress in computer technology, the computer simulation become the most powerful way to predict the morphological change at the transition growth and the characteristic shape at the steady-state growth.

In the last decade, phase-field methods have attracted considerable interest as a means of simulating microstructural development during solidification [2,3]. The phase-field method introduces an auxiliary continuous order parameter ϕ, which takes the constant value in the solid and liquid, with a rapid transition in the vicinity of the solid–liquid interface. The main advantage of the method is that the location of the solid–liquid interface is given implicitly by the phase field. However, since fine meshes are needed to allow continuous and sharp variations of the phase field in small interface regions, considerable computer resources are required when we perform the phase-field simulations using a regular grid, particularly for a large system.

From the viewpoint of numerical calculation, we need not solve the phase-field equation in the bulk phase, because the phase field ϕ is constant inside both liquid and solid. In other words, we need only solve it in the vicinity of the interface. The region in which the phase-field equation must be solved is considerably small, since the area of the solid–liquid interface is generally much smaller than the full computational domain. Adaptive mesh techniques which use fine meshes only around the interface and coarse ones in the bulk phase, therefore, have been successfully applied to the phase-field simulation. Since the method must dynamically adapt the grid to follow the evolving interface, the adaptive method using a fixed grid is more appropriate for reducing the grid operating time and more robust than the deforming grid method often used in structural analysis. The finite difference method [4,5], finite element method [6–10], and finite volume method [11–13] have been applied in the adaptive phase-field simulations.

Recently, the phase-field methods have also been applied to directional solidification [14–20]. The adaptive method could be more appropriate for the directional solidification problem than for the undercooling one, because a large computational domain and a long calculation time are required to evaluate the characteristics of the steady-state growth, such as primary arm spacing, after the planar initial interface becomes unstable and competitive growth occurs between dendritic or cellular arrays.

In this study, phase-field simulations during the directional solidification of a binary alloy are conducted by using the adaptive finite element method. In previous studies for the adaptive phase-field simulation using the finite element method, a triangular [6,7] or a quadrilateral element with an additional triangle element to connect the extra node [8–10] has been used. Here, we introduce the adaptive finite element method only using an isoparametric quadrilateral element, in which the degree of freedom for the extra hanging node which occurs when an element is split into four child elements is eliminated by conducting the matrix operation. The simulations are performed under similar conditions to those of Boettinger [14] and Lan [15], and the effects of the pulling velocity and the temperature gradient on the interface morphology and the primary arm spacing are examined.

2. Simulation method

2.1. Phase-field equations

The thermodynamically consistent phase-field model for a binary alloy based on the entropy functional is adopted here [21,22]. We briefly summarize the used phase-field model in this section [21,22]. In the present simulations during directional solidification, the temperature gradient is assumed to be constant. The phase-field equation and concentration field equation, therefore, must be solved numerically. Considering the effects of anisotropy and noise, the equations in a two-dimensional problem