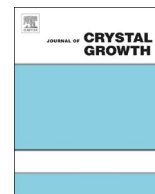




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## Phase-field-lattice Boltzmann studies for dendritic growth with natural convection

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### ABSTRACT

Simulating dendritic growth with natural convection is challenging because of the size of the computational domain required when compared to the dendrite scale. In this study, a phase-field-lattice Boltzmann model was used to simulate dendritic growth in the presence of natural convection due to a difference in solute concentration. To facilitate and accelerate the large-scale simulation, a parallel computing code with multiple graphics processing units was developed. The effects of the computational domain size as well as those of gravity on the dendritic morphologies were examined by performing two-dimensional free dendritic growth simulations with natural convection. The effects of the gravity direction on the dendrite spacing and morphology were also investigated by simulating unidirectional solidification from multiple seeds.

### 1. Introduction

Solidification is a complicated multi-physics phenomenon that includes the migration of the solid-liquid interface, thermal and solute diffusions, and the flowing of the melt [1]. In particular, the melt flow drastically changes the solidification microstructures [2–4]. Recently, Shevchenko et al. performed a series of in-situ observations during the directional solidification of an In–Ga alloy [5–11] and uncovered interesting phenomena, such as plume flow; unusual overgrowth where the largely inclined dendrites overgrew the dendrites oriented favorably with respect to the heat flow direction; and freckle formations, which were caused by the natural convection initiated by the difference in the densities between In and Ga. The freckle, or channel-type segregation, is a typical solidification defect [12–14]. A few numerical studies have been performed on the solidification of pure metals and alloys accompanying natural convection, in order to determine the freckle formation mechanism and criteria [14–19]. However, these simulations focused on macrosegregation, and the effects of the microstructures were introduced by means of empirical parameters, such as the mushy zone permeability and the dendritic spacing during directional solidification. Recently, Saad et al. [20] developed a channel-segrega-

tion prediction model at the grain scale by coupling the cellular automaton and finite element methods [21,22]. The simulated solidification morphologies were found to be in good agreement with the in-situ observations of the In–Ga alloy solidification process [7]. Karagadde [23], Yuan [24,25], and Kao [26] simulated dendritic growth with natural convection at the dendrite scale using a cellular automaton technique. They could observe the interaction between dendritic growth and melt flow in the mushy zone and succeeded in elucidating freckle formation. However, the accuracy of the dendritic morphology was insufficient.

The phase-field method is a numerical model that can simulate dendritic growth with high accuracy [27–30]. The phase-field method has been applied successfully to study dendritic growth with melt convection [31,32]. While a number of phase-field studies have focused on forced convection [31,33–46], there have been few studies on dendritic growth with natural convection [47–50]. To the best of our knowledge, only Apel [47] and Steinbach [50] have investigated the growth of multiple dendrites with natural convection. The reason for this lack of phase-field studies on dendritic growth with natural convection is that solidification simulations involving natural convection require a much larger computational domain compared to the

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dendrite scale. Therefore, the key is to develop a large-scale phase-field simulation technology for high-accuracy predictions of material microstructures. General-purpose computing on graphics processing units (GPGPU) has emerged as a promising large-scale simulation trend in computational materials science [29,51–64]. We have been able to successfully perform parallel GPU-based large-scale phase-field simulations using the GPU-rich supercomputer TSUBAME2.5 at the Tokyo Institute of Technology [29,52,54–58,63,64].

In this study, to allow for an accurate and large-scale simulation of dendritic growth in the presence of natural convection, we develop a parallel GPU code for a model that combines the phase-field and lattice Boltzmann methods. The effects of the computational domain size and gravity on the dendrite morphology are investigated in detail. Here, as a first step toward studying dendritic growth with natural convection, we focus on the large-scale simulations of the two-dimensional isothermal solidification of a binary alloy.

## 2. Phase-field-lattice Boltzmann model

Recently, we developed a phase-field-lattice Boltzmann model that can simultaneously simulate dendritic growth, dendritic motion, and melt convection during the isothermal solidification of a binary alloy [51,65]. In this model, the dendritic growth, melt flow, and dendritic motion are simulated by the quantitative phase-field model [66], the lattice Boltzmann method [67], and using the equations of motion, respectively. In this study, the model is applied to dendritic growth with natural convection. For simplicity, the problem is restricted to two-dimensional isothermal solidification without the motion of the dendrite. The phase-field method is the most accurate numerical model for simulating dendrite growth and is easily discretized by the normal finite difference method. It is easier to implement the lattice Boltzmann model than it is to directly solve the Navier–Stokes equations. Further, the method is suitable for parallel computations. That is to say, a coupling model based on the phase-field and lattice Boltzmann methods is suitable for high-accuracy large-scale parallel computations.

### 2.1. Quantitative phase-field model

The isothermal solidification of a dilute binary alloy can be simulated by the quantitative phase-field model developed by Ohno and Matsuura [66]. In this model, we use two variables: the phase-field,  $\phi$ , and the non-dimensional supersaturation,  $u$ . The phase-field is defined as  $\phi = +1$  in the solid and  $\phi = -1$  in the liquid and changes smoothly within the solid–liquid interface region. The non-dimensional supersaturation is defined by  $u = (C_l - C_l^e)/(C_l^e - C_s^e)$ , where  $C_l$  is the concentration in the liquid, and  $C_l^e$  and  $C_s^e$  are the equilibrium concentrations in the liquid and solid, respectively. We employ the relation  $k = C_s^e/C_l^e = C_s/C_l$  by following the Kim–Kim–Suzuki (KKS) model [68], where  $k$  is the partition coefficient. Then, the concentration,  $C$ , is given as  $C = C_s(1+\phi)/2 + C_l(1-\phi)/2$ . The time evolution equations of  $\phi$  and  $u$  can be expressed as follows:

$$\begin{aligned} \tau(\theta) \frac{\partial \phi}{\partial t} &= \nabla \cdot (W(\theta)^2 \nabla \phi) - \frac{\partial}{\partial x} \left[ W(\theta) \frac{\partial W(\theta)}{\partial \theta} \frac{\partial \phi}{\partial y} \right] + \frac{\partial}{\partial y} \left[ W(\theta) \frac{\partial W(\theta)}{\partial \theta} \frac{\partial \phi}{\partial x} \right] \\ &\quad - \frac{df(\phi)}{d\phi} - \lambda^* \frac{dg(\phi)}{d\phi} u, \end{aligned} \quad (1)$$

$$\begin{aligned} \frac{1}{2} [1 + k - (1 - k)\phi] \left( \frac{\partial u}{\partial t} + \mathbf{U} \cdot \nabla u \right) &= \nabla [D_l q(\phi) \nabla u - \mathbf{J}_{AT}] \\ &\quad + \frac{1}{2} [1 + (1 - k)u] \frac{\partial \phi}{\partial t} - \nabla \cdot \mathbf{J}. \end{aligned} \quad (2)$$

In Eq. (1), we take into account the two-dimensional crystalline anisotropy of the interface energy and the phase-field kinetics by expressing the phase-field relaxation time,  $\tau$ , and the interface thick-

ness,  $W$ , as  $\tau(\theta) = \tau_0 a_s(\theta)^2$  and  $W(\theta) = W_0 a_s(\theta)$ , respectively, where  $\tau_0$  and  $W_0$  are the standard values of  $\tau$  and  $W$ . We employ  $a_s(\theta) = 1 + \varepsilon_4 \cos(4\theta)$  as the anisotropy function with four-fold anisotropy, where  $\theta$  is the angle between the  $x$ -axis and the interface normal and  $\varepsilon_4$  is the anisotropy strength. Then  $\lambda^*$  is a coupling constant associated with the thermodynamic driving force, which is expressed as  $\lambda^* = a_1 W_0 / d_0$ , where  $a_1$  is a constant and  $d_0$  is the chemical capillary length defined by  $d_0 = \Gamma / (|m|(1-k)c_l^e)$ , with  $\Gamma$  the Gibbs–Thomson constant and  $m$  the liquidus slope. The standard relaxation time,  $\tau_0$ , is expressed by  $\tau_0 = a_2 \lambda^* W_0^2 / D_l$ , where  $a_2$  is a constant and  $D_l$  is the diffusion coefficient in the liquid. The constants  $a_1$  and  $a_2$  are determined when choosing the functions  $f(\phi)$  and  $g(\phi)$ ; here, we use  $a_1 = 0.8839$  and  $a_2 = 0.6267$  for  $df(\phi)/d\phi = -\phi + \phi^3$  and  $dg(\phi)/d\phi = (1 - \phi^2)^2$  [69]. In Eq. (2),  $\mathbf{J}_{AT}$  is an antitrapping current expressed as  $\mathbf{J}_{AT} = -(1 - k D_s / D_l) / (2\sqrt{2}) W_0 [1 + (1 - k)u] [\partial \phi / \partial t] \nabla \phi / |\nabla \phi|$  using the diffusion coefficients in the solid,  $D_s$ , and the liquid,  $D_l$ . In addition,  $\mathbf{J}$  is the fluctuating current [70] and  $q(\phi)$  is an interpolation function expressed as  $q(\phi) = [k D_s + D_l + (k D_s - D_l)\phi] / (2D_l)$ . An advection term is added to the original diffusion equation [66], in order to express the solute flow driven by the fluid velocity,  $\mathbf{U}$ , as determined by the lattice Boltzmann method.

### 2.2. Lattice Boltzmann model

The fluid velocity is computed by the lattice Boltzmann method [67]. The advantage of employing the lattice Boltzmann method is its suitability for parallel computation because there is no need to solve the Poisson's equation in the Navier–Stokes equations. The lattice Boltzmann equation while considering the discrete force  $G_i$  can be expressed as

$$f_i(\mathbf{x} + \mathbf{c}_i \delta t, t + \delta t) = f_i(\mathbf{x}, t) - \frac{1}{\tau_{LBM}} [f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)] + G_i(\mathbf{x}, t) \delta t, \quad (3)$$

where  $f_i$  is the particle velocity distribution function in the  $i$ -th discrete direction,  $f_i^{eq}$  is the equilibrium distribution function,  $\tau_{LBM}$  is the single relaxation time,  $\mathbf{c}_i$  is the discrete particle velocity,  $\mathbf{x}$  is the position vector,  $t$  is the time,  $\delta t$  is the time step size, and  $G_i$  is the discrete external force. The equilibrium distribution function,  $f_i^{eq}$ , is expressed as

$$f_i^{eq} = \rho w_i \left[ 1 + \frac{3(\mathbf{c}_i \cdot \mathbf{U})}{c^2} + \frac{9(\mathbf{c}_i \cdot \mathbf{U})^2}{2c^4} - \frac{3\mathbf{U} \cdot \mathbf{U}}{2c^2} \right], \quad (4)$$

where  $w_i$  is the weight function and  $c$  is the lattice velocity. The discrete external force,  $G_i$ , is given by

$$G_i = \rho w_i \left[ 3 \frac{\mathbf{c}_i \cdot \mathbf{U}}{c^2} + 9 \frac{(\mathbf{c}_i \cdot \mathbf{U}) \mathbf{c}_i}{c^4} \right] \cdot (\mathbf{G}_D + \mathbf{G}_B), \quad (5)$$

where  $\mathbf{G}_D$  is the dissipative drag force vector to satisfy the no-slip boundary condition at the solid–liquid interface [31]:

$$\mathbf{G}_D(\mathbf{x}, t) = -\frac{2\rho\nu h}{W_0} \left( \frac{1 + \phi}{2} \right)^2 \mathbf{U}. \quad (6)$$

Here,  $\nu$  is the kinematic viscosity and  $h$  is a constant and equal to 2.757 [31]. The buoyancy force due to the concentration difference in the liquid is given by

$$\mathbf{G}_B(\mathbf{x}, t) = -\rho g \beta_C (C - C_0) \frac{1}{2} (1 - \phi), \quad (7)$$

where  $\mathbf{g}$  is the gravity acceleration vector,  $\beta_C$  is the solute expansion factor, and  $C_0$  is the initial liquid concentration. The introduction of Eq. (7) is a novel point with respect to the previous model [65]. The density,  $\rho$ , and fluid velocity,  $\mathbf{U}$ , are computed using

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