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Phase-field lattice Boltzmann simulations of multiple dendrite growth with motion, collision, and coalescence and subsequent grain growth

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ABSTRACT

In the formation of a typical equiaxed structure during the solidification of metals and alloys, multiple equiaxed dendrites typically grow with motion, collision, and coalescence and subsequently grain growth occurs after the formation of grain boundaries. In this study, we develop a phase-field lattice Boltzmann model that can simulate these complex formation processes involving equiaxed structures. In this model, multiple dendrites are represented by employing multiple phase-field variables, and the formation of grain boundaries is modeled by simply introducing an interaction term between the phase-field variables. Liquid flow is computed using the lattice Boltzmann method, and the motion of a solid is described by solving the equations of motion. Collision-coalescence representation in the present model was validated by performing simulations of collisions between two circular objects. Furthermore, grain growth was validated through static and dynamic conditions in a simple three-grain system. Good agreements with theoretical solutions were obtained for both cases. Finally, using the developed model, a series of formation processes of multiple-dendrite growth with motion, collision, and coalescence and the subsequent grain growth are successfully performed for the first time.

1. Introduction

A typical solidification structure consists of columnar and equiaxed polycrystalline structures [1–3]. It is essential to accurately control and predict the equiaxed structures, especially because they determine the mechanical and other properties of the cast materials. In the formation process of an equiaxed structure, the solids nucleate in a supercooled liquid and they grow into equiaxed dendrites. Importantly, they move in the liquid as a result of forced convection caused by pouring and/or natural convection due to the difference in density between the solid and liquid. During growth of equiaxed dendrites, therefore, they collide with each other and coalesce into a single solid particle. The grain boundaries are then formed and grain growth begins. Finally, the entire region becomes a polycrystalline solid and grain growth proceeds.

The formation of an equiaxed structure has been simulated using a phase-field method [4], which is the most accurate model for describing dendritic growth, in both two dimensions (2D) [5,6] and three dimensions (3D) [7,8]. In such simulations, the motion of dendrites was not taken into account. Because the melt convection necessarily occurs in terrestrial solidification, the isolated equiaxed dendrites can move [9–12]. Considering this fact, some studies on dendritic growth with motion have been presented in recent years [13–18]. Rojas et al. succeeded in modeling this phenomena by coupling the phase-field method, lattice Boltzmann method, and equations of motion [15]. Besides, through accelerated computations of the model using a graphical processing unit (GPU), Takaki et al. showed that the model can simulate the long-distance motion of growing dendrite with rotation [17]. Although good predictions have been obtained, this model focus on the growth of a single dendrite. Thus, Qi et al. modeled the multiple dendrite growth with motion [18]. A more realistic situation, however, involves the interaction of multiple dendrites undergoing growth, motion, collision, coalescence, and the subsequent grain growth. This complex equiaxed polycrystalline microstructure has not been predicted so far.

In this study, by extending the model developed by Rojas et al. [15] to multiple dendrites, we develop a new phase-field lattice Boltzmann model that can describe the formation process of an

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equiaxed polycrystalline structure with growth, motion, collision, and coalescence of multiple dendrites and subsequent grain boundary formation and grain growth.

2. Model

In this study, a 2D isothermal solidification of a binary alloy is assumed unless otherwise stated. The dendrite growth and subsequent grain growth are modeled using the phase-field method [19,20], the liquid flow is computed using the lattice Boltzmann method, and the motion of a solid is expressed by the equations of motion. The combination of these models has some advantages including the easy implementation on Cartesian grids and the capability of parallel computation.

2.1. Phase-field method

A polycrystalline structure is expressed by N phase-field variables ϕ_i, which are defined as $\phi_i = +1$ in the i-th grain and $\phi_i = -1$ in the other grains and change smoothly at the interface region. At the solid–liquid interface, the time evolution equation of ϕ_i expressing the i-th solid grain is expressed as [19]:

$$\tau(\theta_i)\frac{\partial\phi_i}{\partial t} = \nabla(W(\theta_i)^2\nabla\phi_i) - \frac{\partial}{\partial x}\left[W\frac{dW(\theta_i)}{d\theta_i}\frac{\partial\phi_i}{\partial y}\right] + \frac{\partial}{\partial y}\left[W(\theta_i)\frac{dW(\theta_i)}{d\theta_i}\frac{\partial\phi_i}{\partial x}\right] - (-\phi_i+\phi_i^3) - \lambda^*(1-\phi_i^2)^2 u, \tag{1}$$

where τ is the phase-field relaxation time, W is the interface thickness, λ^* is a parameter associated with the thermodynamic driving force, and u is the non-dimensional supersaturation. The terms τ and W are functions of crystal orientation θ_i expressed as $\tau(\theta_i) = \tau_0 a_s(\theta_i)^2$ and $W(\theta_i) = W_0 a_s(\theta_i)$, respectively. Here, the anisotropic function was set to $a_s(\theta_i) = 1 + \varepsilon_4\cos(4\theta_i)$, where ε_4 is the strength of anisotropy. The change in θ_i occurs due to the rotation of the dendrite and is updated during the simulation. At the solid–solid grain boundary and the higher-order junctions, such as the triple junction, the following equation is solved:

$$\tau_0\frac{\partial\phi_i}{\partial t} = W_0^2\nabla^2\phi_i - (-\phi_i+\phi_i^3) + \chi_i. \tag{2}$$

Here, it is assumed that the energy and mobility of the grain boundaries are the same as the average values of the solid–liquid interface. In Eq. (2), i takes a value from 0 to N, and the 0th phase-field variable, ϕ_0, represents the liquid phase. The term χ_i is the interaction term between the multiple phase-field variables, and it is derived to satisfy the relation $\sum_{i=0}^{N}\frac{1}{2}(\phi_i+1) = 1$. By differentiating this relation with respect to time t, we obtain $\sum_{i=0}^{N}\frac{\partial\phi_i}{\partial t} = 0$. By substituting Eq. (2) into this equation, we get:

$$\sum_{i=0}^{N}\chi_i = -\sum_{i=0}^{N}\left[W_0^2\nabla^2\phi_i - (-\phi_i+\phi_i^3)\right]. \tag{3}$$

Finally, the *following* form proposed by Lee and Kim [20] to satisfy Eq. (3) is employed:

$$\chi_i = -\frac{(\phi_i+1)^2}{\sum_{j=0}^{N}(\phi_j+1)^2}\sum_{j=0}^{N}\left[W_0^2\nabla^2\phi_j - (-\phi_j+\phi_j^3)\right]. \tag{4}$$

The non-dimensional supersaturation u is defined by $u = (C_l - C_l^e)/(C_l^e - C_s^e)$, where C_l^e and C_s^e are the equilibrium concentrations of the liquid and solid, respectively. We employed the relations $k = C_s^e/C_l^e = C_s/C_l$ for the concentrations of the liquid and solid, C_l and C_s [21]. Therefore, the concentration C is given as $C = C_s(1+\phi)/2 + C_l(1-\phi)/2$. The evolution equation of u is given by:

$$\frac{1}{2}[1+k-(1-k)\phi_s]\left(\frac{\partial u}{\partial t} + \mathbf{U}\cdot\nabla u\right) = \nabla[D_l q(\phi)\nabla u - \mathbf{J}_{AT}] + \frac{1}{2}[1+(1-k)u]\frac{\partial\phi_s}{\partial t} - \nabla\cdot\mathbf{J}, \tag{5}$$

where $\mathbf{J}_{AT}$ is an antitrapping current expressed as $\mathbf{J}_{AT} = -(1 - kD_s/D_l)/(2\sqrt{2})W_0[1+(1-k)u](\partial\phi_s/\partial t)\nabla\phi_s/|\nabla\phi_s|$ with D_s and D_l representing the diffusion coefficients of the solid and liquid, respectively. ϕ_s is the phase-field variable expressing the solid phase, or $\phi_s = -\phi_l = -\phi_0$, because the 0th phase-field variable is set to express the liquid phase. In addition, $\mathbf{J}$ is the fluctuating current [22] and $q(\phi)$ is an interpolating function expressed as $q(\phi_s) = [kD_s + D_l + (kD_s - D_l)\phi_s]/(2D_l)$. In Eq. (4), $\mathbf{U}$ is the fluid velocity computed by the lattice Boltzmann method.

2.2. Lattice Boltzmann method

The lattice Boltzmann equations used in this study are identical to those developed by Rojas et al. [15]. The lattice Boltzmann equation is expressed as:

$$f_k(\boldsymbol{x}+\mathbf{c}_k\delta t, t+\delta t) = f_k(\boldsymbol{x},t) - \frac{1}{\tau_{LBM}}\left[f_k(\boldsymbol{x},t) - f_k^{eq}(\boldsymbol{x},t)\right] + G_k(\boldsymbol{x},t)\delta t, \tag{6}$$

where f_k is the particle velocity distribution function in the discretized k-th direction, f_k^{eq} is the equilibrium distribution function, τ_{LBM} is the single relaxation time, $\mathbf{c}_i$ is the discrete particle velocity, $\boldsymbol{x}$ is the position vector, t is the time, δt is the time step size, and G_k is the discrete external force. The equilibrium distribution function f_k^{eq} is expressed as:

$$f_k^{eq} = \rho w_k\left[1 + \frac{3(\mathbf{c}_k\cdot\mathbf{U})}{c^2} + \frac{9(\mathbf{c}_k\cdot\mathbf{U})^2}{2c^4} - \frac{3\mathbf{U}\cdot\mathbf{U}}{2c^2}\right], \tag{7}$$

where w_k is the weight function and c is the lattice velocity. The discrete external force G_k is given by:

$$G_k = \rho w_k\left[3\frac{\mathbf{c}_k - \mathbf{U}}{c^2} + 9\frac{(\mathbf{c}_k\cdot\mathbf{U})\mathbf{c}_k}{c^4}\right]\cdot\mathbf{G}, \tag{8}$$

where $\mathbf{G}$ is the dissipative drag force vector satisfying the no-slip boundary condition at the solid–liquid interface [23]:

$$\mathbf{G}(\mathbf{x},t) = -\frac{2\rho\nu h}{W_0}\left(\frac{1+\phi_s}{2}\right)^2(\mathbf{U} - \mathbf{U}_{S\alpha}). \tag{9}$$

Here, ν is the kinetic viscosity, h is a constant equal to 2.757, and $\mathbf{U}_{S\alpha}$ is the α-th solid velocity vector determined by the equations of motion. The density ρ and fluid velocity $\mathbf{U}$ are computed, respectively, using:

$$\rho = \sum_{k=0}^{Q-1} f_k \text{ and} \tag{10}$$

$$\rho\mathbf{U} = \sum_{k=0}^{Q-1}\mathbf{c}_k f_k, \tag{11}$$

where Q is the number of discrete velocities. In the following simulations, the D2Q9 model is used, which denotes a 2D problem and $Q = 9$.

Note that all the parameters in this section are dimensionless values, *i.e.*, the length, time, and velocity are normalized by the dimensional lattice size Δx, the time increment Δt, and the velocity $\Delta x/\Delta t$, respectively. Therefore, the lattice size δx and δt are rescaled to unity as $\delta x = 1$ and $\delta t = 1$.