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Phase field modeling of lamellar eutectic growth under the influence of fluid flow

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ABSTRACT

Using PF-LBM (phase-field and Lattice-Boltzmann) model, the effects of flow velocity and flow direction on the CBr_4-C_2Cl_6 eutectic lamellar growth morphology in the forced flow are simulated and studied. The results show: the liquid flow direction and flow velocity have significant influence on morphology of eutectic lamellar growth; without liquid flow, the lamellar growth mode is symmetrical growth mode, which is perpendicular to the solid-liquid interface; with flow velocity u = 0.005 m/s, when the angle Θ = 0° which between the liquid flow direction and the Y direction (parallel to the eutectic lamellar), liquid flow hasn't effect on eutectic growth morphology; when the angle Θ = 45°, the simulation time t = 20,000Δt, the lamellar growth mode is the mode of oscillation, the β phase nucleation and the α lamellar branching in the front of interfaces; when the angle Θ = 90°, the simulation time t = 40,000Δt, the lamellar growth mode is the mode of eutectic lamellar spacing oscillation and grows to liquid flow direction, and the interface of the lamellar is not steady, which couples with the β phase nucleation and the α phase branching; when the angle Θ = 45°, the simulation time t = 120,000Δt, the complex growth morphology of eutectic lamellar spacing oscillation, the β phase nucleation and the α phase branching appear in the front of interfaces; when the angle Θ = 90°, the simulation time t = 120,000Δt, the steady growth of the initial oscillation and the growth mode of the β phase nucleation and the α phase lamellar branching (when t = 40,000Δt) are maintained; in contrast to the angle Θ = 90°, when the angle Θ = 45°, the phenomenon of lamellar spacing decreases and lamellar pairs increase earlier appear because of the spacing adjustment. when the angle Θ = 90°, with the increase of the flow velocity, the growth velocity of lamellar eutectic is faster, and growth toward the liquid flow direction is more obvious; when flow velocity u = 0.0 m/s (without flow field), the lamellar growth morphology is the growth pattern of oscillation and symmetry, which is perpendicular to the solid-liquid interface; when flow velocity u = 0.003–0.005 m/s, the lamellar growth morphology is the mixed growth pattern of oscillation and tilting to the liquid flow direction; when flow velocity u = 0.007–0.009 m/s, the lamellar growth morphology is the steady mode of lamellar spacing decreases and lamellar pairs increase in the front of interface because of the β phase nucleation. With the increase of flow velocity, the lamellar morphology selection is: eutectic lamellar spacing symmetrical oscillation state, which is perpendicular to the solid-liquid interface → tilt growth and lamellar spacing oscillatory instability → lamellar spacing oscillation the β phase nucleation and the α phase branching in the front of lamellar interface.

1. Introduction

Eutectic lamellar morphology is one of the common microstructures during solidification of eutectic alloys [1,2]. The morphology and structure of eutectic microstructure have a great influence on the mechanical properties of materials [3]. Phase field method, as an important simulation method, which is an efficient tool to study complex microstructure morphology [3], and makes researchers can simulate directly the formation of microstructure.

The phase field method has emerged as a powerful tool to simulate the structure and morphology of eutectic microstructure in the past 20 years, which is getting more and more mature [4–17]. As the development of modern science and technology, phase field simulation research of eutectic microstructure has expanded from two-dimensional (2D) [18–22] to three-dimensional (3D) [23–27], and from binary alloys to multi-alloys [23]. Li

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Shengjian [18] and Nestler [19] studied study the lamellar stability of a directionally solidified hypereutectic CBr_4-C_2Cl_6 alloys by using the multiphase field model in 2D; LI [20] studied the relationships between lamellar spacing and choices of the eutectic growth morphology during solidification of eutectic alloys by using the phase field model in 2D; Choudhury [21] studied the self-organization formation for ternary eutectic alloy (Ag-Al-Cu) during the solidification by using the phase field model in 2D; Apel [22] studied the morphology selection mechanism for both lamellar and rod-like in 2D and 3D by using the phase field model; Yang Yu Juan [23–27] studied the growth morphological evolution and the transition mechanism of CBr_4-C_2Cl_6 eutectic alloy during the unidirectional solidification in 3D by using the phase field model. Fluid flow always exist in the solidification from a melt, which has an important effect [28]on the formation of microstructures and on the properties of materials. The effect of flow field on eutectic lamellar spacing and peritectic for a Cu-Al alloy were studied qualitatively using the phase field model by Nestler [29] in 2D; Chen [30] studied the influence of liquid flow velocities on the eutectic growth during the directional solidification. In the above research works, the simulation results of lamellar eutectic growth are almost qualitative and two-dimensional. Selzer [31] studied qualitatively the influence of flow field on the rod growth for Al-Cu eutectic alloys in 3D with the LBM model. Summary of the existing research reports, three dimensional eutectic lamellar growth is less in the phase field method coupled with flow field aspect.

In this paper, we take the transparent CBr_4-C_2Cl_6 for example, to analyze the influence of flow velocity and flow direction on the growth of eutectic lamellar microstructures, we apply the coupled phase-field and Lattice-Boltzmann model for numerical simulations.

2. Phase-field model

2.1. Multi-phase field governing equations

The eutectic phase field governing equation of KKSO multi-phase field model [32]

$$\frac{\partial \phi_i}{\partial t} = \frac{-2}{n} \sum S_{ij} M_{ij} \left[\frac{\delta F}{\delta \phi_i} - \frac{\delta F}{\delta \phi_j} \right] \tag{1}$$

where

$$\frac{\delta F}{\delta \phi} = \sum_{j \neq i} \left[\frac{\varepsilon_{ij}}{2} \nabla^2 \phi_j + \omega_{ij} \phi_j \right] + f^i(c_i) - c_i f_c \tag{2}$$

where ϕ_i is phase field, respectively respects volume fractions of each phase; $n = \sum_{i=1}^{3} s_i$, $s_{ij} = s_i s_j$, s_i is step function; M_{ij} is the kinetic coefficient of phase field; ε_{ij} is the gradient energy coefficient; ω_{ij} is the height of the double-well potential; f is the free energy densities; c is the compositions of each phase.

The diffusion equation where the mass should be conserved is written as:

$$\frac{\partial c}{\partial t} = \nabla \cdot D \sum_i \phi_i \nabla c_i \tag{3}$$

where D is the solute diffusion coefficient.

2.2. The concentration diffusion governing equation of coupling with flow field

After coupling with flow field, the comprehensive effect of solute redistributions, solute diffusion and fluid flow velocities on solute distributions during the process of solidification. Eq. (3) is add to the influence part of flow field, which is

$$\frac{\partial c}{\partial t} = \nabla M_c \nabla \frac{\delta F}{\delta c} - \nabla (u \cdot c) \tag{4}$$

where c is the composition; t is time variables; u is the flow velocity; M_c is the kinetic coefficient of concentration diffusion field; F is the volume free energy of system.

2.3. LBM governing equation of fluid field

LBM model is a model of fully discrete local dynamics, which makes fluid simple into lots of particles, those particles happen collision and move on every point of grid. The evolution equation of particle distribution in LBM algorithm is

$$f_i(x + c_i \Delta t, t + \Delta t) = f_i(x, t) + \Omega_i(f(x, t)) \tag{5}$$

where $f_i(x,t)$ is the velocity distribution function of i direction particles in X at t time; $\Omega_i(f(x,t))$ is i direction of the particle collision function, in this paper, the LBGK model in which the expression is:

$$\Omega_i(f(x,t)) = \frac{1}{\tau} [f_i(x,t) - f_i^{eq}(x,t)] \tag{6}$$

where $f_i^{eq}(x,t)$ is particle distribution function on balance condition; τ is relaxation time.

In LBM model, particle distribution function on balance condition is:

$$\begin{cases} f_i^{eq} = \rho \omega_i \left[1 + \frac{c_i \cdot \boldsymbol{u}}{c_{sm}^2} + \frac{(c_i \cdot \boldsymbol{u})^2}{2c_{sm}^4} - \frac{\boldsymbol{u}^2}{2c_{sm}^2} \right] \\ c_{sm} = c_m / \sqrt{3} \end{cases} \tag{7}$$

where u is the flow velocity; ρ is the local fluid density; ω_i is weighting function if i = 0, $\omega_i = 1/3$, if i = 1–6, ϕ_i=1/18, if i = 7–18, $\omega_i = 1/36$; c_i is particle discrete velocity; c_m is grid nodes velocity.

3. Computational conditions

3.1. The initial condition and boundary condition

The initial condition is constructed by putting alternating α and β with equilibrium volume fractions. In order to reduce computational complexity, only two pairs of lamellae are set as the initial condition, and the lamellar width w is twice as the initial lamellar spacing λ (w = 2) that have been proposed in all 3D simulations. An adiabatic boundary condition is imposed on the system boundaries perpendicular to the flow direction, while a periodic condition on the other two boundaries. In process of the simulation, the initial eutectic lamellar is introduced in the bottom of the calculation area with the minimum-undercooling lamellar spacing $\lambda_{\min}$ [33] as the reference. In the paper, the dimensionless initial lamellar spacing is defined as $N = \lambda / \lambda_{\min}$. In the calculation domain, the step space $\Delta x = \Delta y = \Delta z = 0.2$ μm [34], time step $\Delta t = 10.04 \times 10^{-5}$ s, Δt depends on the partial differential equation of the phase field and the stability of the partial differential equation of the solute field in the solving process, Δt meet the following conditions in 3D simulations.

$$\Delta t_1 \leqslant \frac{(\Delta x)^2}{6 M_{ij} \varepsilon_{ij}^2} \tag{8}$$

$$\Delta t_2 \leqslant \frac{(\Delta x)^2}{6 D_L^2} \tag{9}$$

$$\Delta t = 0.9 Min\{\Delta t_1, \Delta t_2\} \tag{10}$$