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Quantitative cellular automaton model and simulations of dendritic and anomalous eutectic growth

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ABSTRACT

A quantitative cellular automaton (CA) model for dendritic and anomalous eutectic growth has been developed. Solid/liquid(SL) interface curvature plays an important role on the dendritic and eutectic growth kinetics. In order to improve the accuracy of calculated interface curvature, a height function method was used in this research. Simulation results showed that the precision of the interface curvature has been significantly improved. And the quantitative ability of present CA model has also been improved through the simulations of equilibrium shapes. Using the quantitative CA model, directional solidification of dendritic and eutectic growth has been investigated, as well as the anomalous eutectic growth during laser remelting process. For anomalous eutectic, it is found that the very fine lamellar eutectic growing at much smaller cooling rate is the reason to observe the lamellar to anomalous transition.

1. Introduction

Accurate and efficient numerical models for solidification microstructure evolution are important for solidification science and industry fields. Cellular automaton(CA) model, which has high computational efficiency and relatively simple physical principles, has large potential for scientific and engineering simulations. However, the mesh induced anisotropy in CA model restricts the physical resolution of CA model to a large extent.

Many CA model researches have been focused on the modifications of capture rules, such as the virtual front tracking algorithm [1], a growth anisotropy reduction with diffusion method (GARED) [2], and points CA model [3]. We also presented two types of modified capture rules: the zigzag capture rule [4] and the limited neighbor solid fraction rule [5].

Solid/liquid(SL) interface curvature plays an important role on the dendritic and eutectic growth kinetics. The numerical error on the calculated interface curvature is one of the main origins of the mesh induced anisotropy in CA model. Counting cell method is the most mentioned interface curvature calculation method in CA model. Beltran-Sanchez et al. [6] demonstrated that the counting cell method is mesh dependent. They proposed another method based on the variation of the unit vector normal (VUVN) to the SL interface. We added an bilinear interpolation modification to the VUVN method, which improved the accuracy of VUVN method [4]. Based on the improvement of the VUVN method, we simulated the orientation selection in dendrite growth, in which the mesh induced anisotropy has been reduced to a large extent [5]. Recent developed CA models were also used this type of curvature calculation method [7–10].

Height function method was commonly used in computational fluid dynamics (CFD), where the calculation of surface tension is required in volume of fluid (VOF) model for free surface fluid flow problems. Cummins et al. [11] has compared the accuracy of curvature estimates from three functions: a convolved VOF function, a height function, and a reconstructing distance function in 2005. They concluded that the height function provided superior results. Popinet [12] found that large errors in height function method occur when the interface normal oriented away from the axis directions. Liovic et al. [13] presented a diagonal mesh to improve the height function's accuracy when the interface normal is oriented away from the axis direction.

Despite the numerical study on the height function method, CA simulations of anomalous eutectic growth was also investigated. Anomalous eutectic is an important eutectic microstructure, which is less understood that lamellar eutectic. Experimental observation on anomalous eutectic can be traced to the solidification of metallic alloys from deep undercooled melt in 1960s [14] and recently laser remelting of Ni-Sn powder bed [15]. One of the typical anomalous eutectic morphologies is globular eutectic. Recently, Wei et al. [16] presented a

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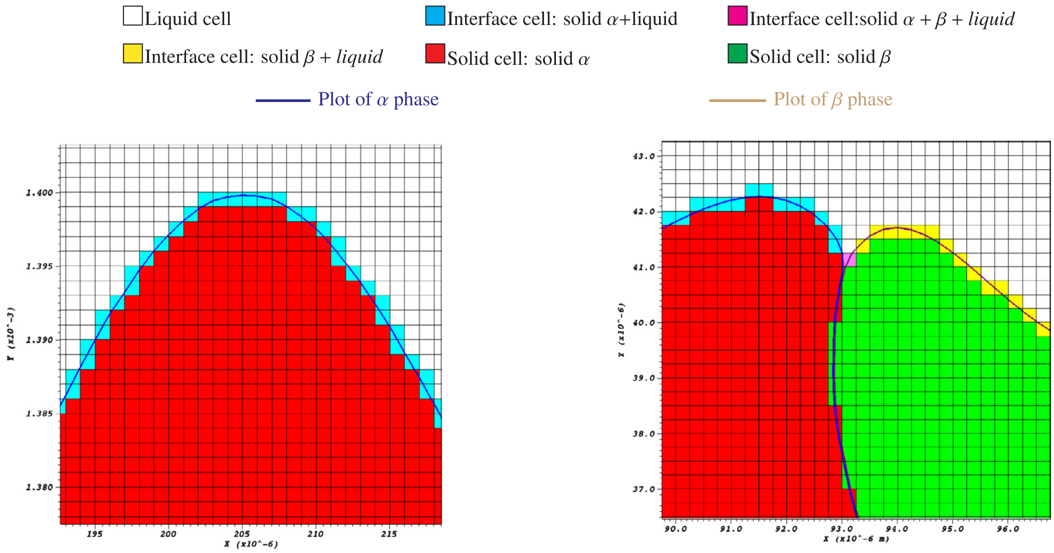

(a) Dendritic growth CA model (b) Eutectic growth CA model

Fig. 1. The definition of cell states in dendritic and eutectic growth CA model.

remelting induced anomalous eutectic growth model based on the eutectic dendrite growth theory. Mullis et al. [17] found out that the volume fraction of anomalous eutectic observed far exceeds the fraction solid that would be expected to form during the recalescence stage of solidification. Anomalous eutectic morphologies were also found at the bottom of melt pool during laser remelting of Ni-Sn eutectic powders once and twice [15]. The EBSD analysis has shown that the remelting of α-Ni dendrites had positive effects on the nucleations of anomalous α-Ni particulates, and also had close relationship with anomalous eutectic morphologies. Up to date, numerical simulation of the anomalous eutectic microstructure evolution is still a great challenge, because the details of anomalous eutectic growth are still unknown. However, the temperature field during laser remelting process could be simplified into directional solidification, which is better understood than that in solidification of deep undercooled melt.

In this paper, the height function method was implemented in CA model to improve the accuracy of interface curvature calculation. Equilibrium shapes were simulated to quantitatively verify the present CA model's mesh induced anisotropy. Simulations of directional solidification of dendritic and lamellar eutectic growth were in agreement with phase field(PF) model and experimental results. With the help of analysis the thermal condition at the bottom of melt pool, the mechanism of anomalous eutectic growth during laser remelting has been investigated, which is a new contribution to the state of the art in anomalous eutectic growth.

2. Mathematic model

In the isothermal solidification process, the growth of SL interface is governed by the diffusion of solute. The boundary conditions at the SL interface is provided by the interface kinetics.

2.1. Solute diffusion

The diffusion of solute is governed by a parabolic differential equation, as seen in Eq. (1).

$$\frac{\partial C_l}{\partial t} = D_l \nabla^2 C_l + C_l(1-k)\frac{\partial f_s}{\partial t} \tag{1}$$

where C_l is the solute composition, D_l is the solute diffusion coefficient, k is the solute partition coefficient, and f_s denotes the fraction of solid in each cell. The second term on the RHS in Eq. (1) is the source term due to the solute rejection effect:

$$C_s = kC_l \tag{2}$$

The solute diffusion in solid phase is neglected in present CA model. The governing equation is solved by an explicit finite difference method.

2.2. Interface kinetics

The interface kinetics in binary alloy CA model is directly related to the local equilibrium condition:

$$T^* = T_l^{eq} + (C_l^* - C_0)m_l - \Gamma K f(\phi, \theta_0) \tag{3}$$

where T^* is the interface temperature, T_l^{eq} is the melting temperature at C_0, m_l is the liquidus slope, C_0 is the initial concentration, Γ is the Gibbs-Thomson coefficient, K is the interface curvature, $f(\phi, \theta_0) = 1 - 15\varepsilon\cos(4(\phi - \theta_0))$, representing the interface energy anisotropy, ϕ is the angle between the interface normal and the x axis, θ_0 is the angle of crystal orientation to the x axis, ε is the interface energy anisotropy coefficient.

For isothermal solidification, the interface equilibrium composition C_l^* is the only unknown variable in Eq. (3). During each time step, the local actual liquid composition of each interface cell C_l is updated to the local equilibrium composition C_l^* [1]. In order to achieve the mass conservation, a quantity of mass is provided, resulting in the increment of solid fraction Δf_s, which is governed by:

$$\Delta f_s = (C_l^* - C_l)/(C_l^*(1-k)) \tag{4}$$

It can be seen that C_l^* is the main factor in interface kinetics. And C_l^* is a function of the interface curvature K and the interface normal ϕ, as seen in Eq. (3). That is the numerical simulation of interface curvature and interface normal determines CA model's quantitative ability, the improvement of which is one of the main contributions in this work.

3. Cellular automaton model

We developed a CA model for isothermal solidification of binary alloy, including dendritic and eutectic growth. The computational domain is divided into Cartesian mesh. For dendritic growth, each mesh (also called cell) should be one of the three states: liquid, interface and solid, as seen in Fig. 1(a). For eutectic growth, it should be one of the six states: liquid, α interface, β interface, α solid, β solid, and three phase