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Low artificial anisotropy cellular automaton model and its applications to the cell-to-dendrite transition in directional solidification

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ABSTRACT

A low artificial anisotropy cellular automaton (CA) model is developed for the simulation of microstructure evolution in directional solidification. The CA model's capture rule was modified by a limited neighbor solid fraction (LNSF) method. Various interface curvature calculation methods have been compared. A modified curvature calculation method based on the variation of the unit vector normal (VUVN) to the solid-liquid interface using volume of fluid (VOF) interpolation technique gets better results. The equilibrium shapes were simulated to quantify the artificial anisotropy, when the interface energy anisotropy coefficient is varied from $\varepsilon = 0.0$ to $\varepsilon = 0.05$. The low artificial anisotropy CA model is used in the numerical simulation of the cell-to-dendrite transition (CDT) in directional solidification. The influence of physical parameters (Γ, D_l, k_0, m_l) on CDT has been investigated. The main finding in this paper is the discovery of the changing behavior of the V_{cd} when the solute partition coefficient k_0 is larger than a critical value. When k_0 is less than 0.125, the V_{cd} follows the Kurz and Fisher criterion V_c/k_0; while when $k_0 > 0.125$, the V_{cd} equals to 8 V_c. The experimental data of succinonitrile-acetone (SCN-ace, $k_0 = 0.1$) and SCN-camphor ($k_0 = 0.33$) support the conclusions from CA simulations.

1. Introduction

The microsegregation between nonplanar solid-liquid interfaces strongly influences the material's mechanical properties. During the directional solidification of alloys, the solid-liquid interface can be a planar, cellular or dendritic morphology, which is depending on the growth conditions (pulling velocity V, thermal gradient G and alloy composition C_0). The instability transition from a planar to a cellular interface at a low velocity and that from a cellular to a planar interface at a high velocity have been established by Mullins-Sekerka instability theory [1]. The cellular interface instability can be cell elimination, tip splitting, or side-branch emission. The side-branch emission, which is also called as the cell-to-dendrite transition (CDT), has remained poorly predicted by theories. Kurz and Fisher's theory [2] predicted that the CDT occurred at $V_{cd} = V_c/k_0$ (V_{cd} = growth velocity of cellular-dendrite transition, V_c = planar growth stability limit, k_0 = solute partition coefficient). Trivedi [3] and Somboonsuk et al. [4] have found that the CDT occurred at the minimum in the solute peclet number, which supported the Kurz and Fisher criterion. Tewari and Laxmanan [5] compared these theories with experimental data from several alloys. It was found that only the V_{cd} in succinonitrile-acetone (SCN-ace) and Al-2%Cu alloys were close to V_c/k_0. Laxmanan suggested that the large variation of V_{cd} may be due to the crystallographic anisotropy effects or the buoyancy convection. Chopra and Tewari [6] showed that the CDT appeared to be strongly influenced by the magnitude of the solute partition coefficient k_0. In their experiments, the V_{cd} in Pb-Sn alloy ($k_0 = 0.5$) was larger than the prediction of the Kurz and Fisher criterion.

Recently, the critical spacing λ_{cd} was introduced into the investigations of the CDT as a control parameter [8–10]. It has been found that the CDT was not sharp. The cell and dendrite coexist in a region of pulling velocities depending on the local spacing. However, the expressions of the critical spacing λ_{cd} presented between Georgelin and Pocheau [8], and Trivedi et al. [9,10] are quite different. Based on the expression of the λ_{cd}, Trivedi et al. also concluded that the CDT initiates when the maximum cell spacing $\lambda_{c,max}$ equals to λ_{cd}. However, the expression of $\lambda_{c,max}$ is still qualitative. Hunt and Lu [11] have presented a rough expression for cell spacing $\lambda_{c,max}$. Phase field simulations [12,14] shown that the maximum finger spacing $\lambda_{c,max}$ was proportion to $1/\sqrt{V}$ (V = the pulling velocity), which was different with the predictions by the Saffman-Taylor

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viscous finger problem [14]. To date, it is still a great challenge to establish the precise expressions of the $\lambda_{c,max}$, $\lambda_{d,min}$ and λ_{cd}, especially considering the influences of the interface energy coefficient ε.

In order to solve the problems mentioned above, numerical simulation is a good option. Numerical model has more control parameters (V, G, C_0, λ, Γ, D_l, k_0, m_l, ε) than that in thin film experiments (V, G, C_0, λ). It is able for the numerical model to quantitatively examine the influences of physical parameters. Phase field model [13,14] has been used to simulate the CDT by controlling the primary spacing, which gave deep understandings of the CDT. Gurevich et al. [14] suggested to give a more exhaustive survey as a function of the various parameters (d_0/l_T, l_D/l_T, Λ/l_T, k_0, and ε), but such a survey remains a nontrivial computational challenge for phase filed model.

A general overview on modeling of primary dendritic solidification microstructure by phase field (PF) and cellular automaton (CA) method can be found in reference [15] and [16], respectively. Compared to the phase field model, CA model has advantages in computational efficiency. The disadvantage of CA model is the artificial anisotropy. The idea of CA was originally introduced by Von Neumann and Burks [17] in 1940s to reproduce complex physical phenomena with simple rules. In 1980s, Wolfram [18] discovered the classic elementary cellular automaton (Rule 110, for instance), which is capable of universal computation. The CA model has highly computational efficiency and relatively simple physical principles. Due to these advantages, CA model has been widely used in simulations of dendrite growth [19–31]. To simulate dendrite growth, Nastac [19] used Von Neumann type of neighborhood definition, the results of which shown strong artificial anisotropy. He also used a counting cell method to calculate the interface curvature. The accuracy of the counting cell method was evidenced to be dependent on mesh size [20]. So far as known, a method based on the variation of the unit vector normal (VUVN) to the solid-liquid interface along the direction of the interface is a better solution [20,21]. However, the VUVN method needs to calculate the derivatives of solid fractions, which is difficult to be accurately calculated in a sharp interface model. The roughness in capture rule definition and curvature calculation are the origin of the artificial anisotropy in CA model.

In order to reduce the artificial anisotropy, there were mainly two kinds of CA models. One was the virtual front tracking method, presented by Zhu and Stefanescu [21]; the second was the decentred square algorithm, presented by Lee and Dong [22,23]. Both of the two methods could make the dendrites grow in arbitrary directions, which was an important improvement. However, there were empirical decision rules in the calculations of interface curvature in the virtual front tracking model. The decentred square algorithm had the disadvantage that the simulated results were still influenced by artificial anisotropy. In recent years, the progressive developments of the CA model were basically based on the two kinds of the CA models. For example, the six symmetrical dendrite growth CA model could be considered as a development of the decentred square algorithm in the hexagonal grid [24]. More importantly, there were some new kinds of CA models. Lorbiecha's PCA model [25], which was based on the randomly distributed CA Points to improve the capture rules and the curvature calculations, achieved the dendrite growth in arbitrary directions. However, it introduced a new problem that the dendritic morphology was not smooth. Marek [26] presented a Growth Anisotropy Reduction with Diffusion method (GARED), which could simulate a dendrite with six fold symmetry on the Cartesian square CA mesh, instead of hexagonal mesh. However, he used kinetic anisotropy instead of interface energy anisotropy. Our previous research provided a zigzag capture rule [27–29] and a limited neighbor solid fraction (LNSF) rule [30]. Both of them were designed to reduce artificial anisotropy. We also introduced a bilinear interpolation algorithm [28] to modify the derivatives of solid fractions in VUVN method. The accuracy of the interface curvature calculation was improved to a large extent. Recently, the quantitative comparison of steady state dendrite tip velocities between the PF and CA models was presented [31]. It was recommended to use a hybrid method, which means that a CA model's outputs are as the inputs of a PF model [32]. However, it is difficult to give a comprehensive comparison between the PF and CA models. Despite the dendrite tip velocities, other solidification morphologies, such as cellular interface [33,34] should also be compared. Unfortunately, due to the artificial anisotropy, most of the CA models' outputs were dendrite morphologies. The cellular and seaweed morphologies in directional solidification require small interface energy anisotropy. CA model has a disadvantage of the precisely describing the morphology of solidification microstructure because of the artificial anisotropy. All kinds of CA models mentioned above didn't have quantitatively examination of the artificial anisotropy by the simulation of the equilibrium shapes.

To date, the PF model is the state-of-the-art numerical model for the simulation of microstructure in solidification process. The PF model implicitly captures the solid-liquid interface, based on the phase-field variable Φ(solid phase for $\Phi = 1$, liquid phase for $\Phi = 0$, interface for $0 < \Phi < 1$). Using the PF variable Φ, it is convenient for the PF model to accurately calculate the interface curvature. By contrast, the interface curvature is difficult to be accurately calculated in the CA model. The CA model, as a sharp interface model, uses a discontinuous Heaviside function of the solid fractions to capture the interface. The interface can be reconstructed by the straightforward SLIC method [37] or by PLIC method [38].

However, the desire of a tracking interface can also be found in the numerical simulation of multiphase computational fluid dynamics (CFD) [39–45]. There were two important approaches for the CFD to capture free interface positions: the volume-of-fluid [39] and the level-set approaches [40]. It can be seen that both of the CA method and the volume-of-fluid approach are sharp interfaces; and both of the PF method and the level-set approach are diffusive interface. In volume-of-fluid approach, the investigations to improve interface curvature have been continuously carried out for decades. Brackbill et al. [42] presented a continuum surface force (CSF) model, in which the volume-of-fluid was convolved with a smoothing kernel. Cummins et al. [43] compared the accuracy of curvature estimates derived from three volume-of-fluid based functions: a convolved volume-of-fluid function (CV), a height function (HF), and a reconstructed distance function (RDF). It was found that the curvature estimates derived from the height function provided superior results. In future work, the CA model can use the latest new curvature estimate method in volume-of-fluid approach, because both of the CA model and volume-of-fluid approach use a discontinuous Heaviside function (the volume fractions) on an Eulerian (fixed) grid to represent the interface.

In this paper, a low artificial anisotropy CA model is developed for the simulation of directional solidification. The influences of physical parameters (Γ, D_l, k_0, $m_l k_0$) on the CDT in directional solidification are investigated by the present low artificial anisotropy CA model.

2. Numerical description of CA model

The computational domain is divided into Cartesian grid. Each grid, which is also called cell, is characterized by three states, such as liquid, solid and interface, as seen in Fig. 1. In order to govern the transition of cell states, a capture rule is needed to control the evolution of different states. Solid fraction (solid cell $f_s = 1$, liquid cell $f_s = 0$, interface cell $0 < f_s < 1$) is introduced to implicitly cap-

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