Numerical simulation of dendritic evolution based on an improved cellular automaton model involving solute field

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Abstract. This paper studied the single crystal growth of Fe-0.64C alloy under a fixed cooling rate, proposed an improved cellular automaton model. The influence of solute field on dendrite growth is especially considered into the model. And a new solute distribution scheme based on Fick’s first law and solute conservation was proposed from the microscopic scale. In addition, the present work improved the acquisition algorithm, which takes the growth length of the interface cell to the neighbouring cell as the determination condition of the capture. A solid fraction calculation method based on the solidification area of interface cell to total area is also proposed. The results show that this model can not only dynamically display the formation process of secondary dendrites and high-order dendrites, but also simulate the distribution of solute inside the dendrites and at the interface front.

1. Introduction

The morphology of the dendrites and the microsegregation formed during the redistribution of the solute play a decisive role in the mechanical properties of the metal. In the traditional process, the trial and error method is used to study the growth of dendrites. Although this method is intuitive, it has blindness, and the workload is large, which wastes manpower and material resources. Otherwise, using computer technology to numerically simulate the dendrite evolution process can avoid a large number of experiments and reduce the research cost. Therefore, since the 1980s, studying the dendritic growth mechanism and using numerical simulation to reproduce the dendrite evolution process has been a hot topic in the field of materials science. The existing research methods are divided into three categories: deterministic methods, phase field methods, and random methods [1-3]. The deterministic model does not conform to the randomness of the nucleation and growth process of the actual solidification process; the phase field method can only simulate small area solidification due to complicated calculation; the MC method in the random method does not consider the details of macroscopic and microscopic transmission, so it lacks a certain physical background; the CA method not only combines the advantages of PF model and MC model, but also has a solid physical basis, which can reflect the influence of solute concentration and undercooling on the solidification process.

Rappaze et al [4,5] first used the CA method in the field of materials science and established a two-dimensional model of dendrites growth from a mesoscopic scale, then optimized the model to establish a three-dimensional model [6]. Based on this, Nastac [7] proposed the Neumann rule, established a fully coupled model of two-dimensional dendrite growth, and randomized the dendrite nucleation process. Zhu et al [8] added the influence of solute redistribution and curvature on the basis of the traditional CA model, improved the phenomenon that the dendrite arm growth deviated from the...
preferred growth direction, and applied this model to the evolution process of three-dimensional dendrites [9,10]. Zhu and Stefanescu [11] proposed a new calculation method of dendrite growth kinetics based on the interface solute balance principle, which obtained secondary and tertiary branches of dendrites. Yin and Wang et al [12,13] considered the influence of flow field on dendrite growth, constructed a lattice Boltzmann (LB-CM) model and a cellular automata lattice Boltzmann (LB-CA), and simulated the phenomenon of forward deflection of dendrites. Artemev et al [14] proposed an improved method for the solute partitioning process. Nakagawa, Chen et al [15-17] used a modified eccentricity algorithm to attenuate the anisotropy brought by the mesh, and simulated the dendritic morphology under different preferred orientations. Kran, Shi et al [18,19] also proposed improvements to attenuate the anisotropy. Luo et al [20] simulated the dendritic growth of Fe-C alloy under convection. In the past two decades, the research on the numerical model of dendrite growth has made great progress, and the accuracy of the model is getting higher and higher, but the mesh anisotropy existing in the modeling process cannot be completely eliminated, and the solute redistribution model during dendrite growth process also lacks systematic and complete analysis.

The actual casting process is very complicated, the liquid metal is cooled under different boundary conditions, then the crystal is driven to nucleate and grow after the melt receiving undercooling. In order to simplify the model and provide the dendrites growth environment, the following assumptions are made on the temperature of dendrites growth environment: the initial undercooling is 1°C, and the cooling rate is 20°C/s. Based on the above assumptions, this paper proposed a new solute distribution scheme, improved the acquisition algorithm and solid fraction calculation method of the cellular automaton model, finally simulated the evolution of dendrites during solidification of a Fe-0.64C alloy with a size of 4 mm×4 mm.

2. Improved cellular automaton model

The present work used an improved cellular automaton model to simulate the evolution of dendrites with temperature field and solute field. In order to simulate secondary and high-order dendrites, the calculation area is divided into 400×400 cells with a size of 10 μm; each cell is given characteristic parameters such as temperature, concentration, preferred orientation and state. Since the dendritic morphology has a four-fold symmetry, the preferred orientation \( \theta \in [-45^\circ, 45^\circ] \), and each cell will undergo a transition of liquid (\( f_s = 0 \)), interface (\( 0 < f_s < 1 \)), solid (\( f_s = 1 \)). All cells are initialized to a liquid state, and a nucleation grain with a preferred orientation \( 0^\circ \) is placed at the central of the calculation region. The process of grain growth in the undercooling melt is accompanied by the discharge of solute, the solute is enriched at the front edge of the solid-liquid interface, which lowers the melting point temperature and reduces the undercooling of the melt, eventually leading to a decrease in the growth rate of dendrites. The cooling rate in the dendrite growth process was assumed to be a fixed value. The new solute distribution model is based on Fick's first law and mass conservation, which makes a comprehensive analysis of the excess solute emissions at the interface front. In addition, the present model proposed new calculation methods for the capture and solid fraction, see details in Section 3. The mechanism of dendritic growth and solute transport in the model are introduced as follows.

2.1. Growth Kinetics equation

In the actual casting process, the undercooling is affected by the diffusion of solute, heat and curvature of the interface. The total undercooling of the interface is a combination of various undercooling:

\[
\Delta T = \Delta T_k - \Delta T_r - \Delta T_c + \Delta T_p
\]

\( \Delta T_k, \Delta T_r, \Delta T_c, \) and \( \Delta T_p \) are kinetic, curvature, solute, thermal and pressure undercooling, respectively. During the growth of dendrites, the kinetic undercooling is generally in the order of 0.01 K~0.05 K, and the effect of pressure undercooling on the equilibrium temperature is also very small.
Therefore, in order to simplify the model, this paper ignores the two kinds of undercooling and established kinetics model:

$$\Delta T = \Delta T_r - \Delta T_f - \Delta T_c$$  \hspace{1cm} (2)

The KGT [21] model was used to establish the relationship between the growth speed of the dendritic tip and the undercooling:

$$v = \alpha \Delta T^2 + \beta \Delta T^3$$  \hspace{1cm} (3)

Growth coefficients $\alpha$ and $\beta$ can be obtained by experimental regression.

2.2. Solute distribution model

It can be seen from the equation (2) that the solute undercooling is an important component of the total undercooling of the melt and it has a great influence on the growth of the dendrites. The traditional CA model ignores the solute field, which inevitably affects the morphology of the dendrites. Therefore, this model specifically incorporates the influence of the solute field. Since the diffusion coefficient of the solid is 3 to 4 orders of magnitude smaller than that of the liquid, the solid solute diffusion is ignored, and only the diffusion of the solute in the liquid and the interface cell is considered. Since the diffusion coefficient of the solid phase is 3 to 4 orders of magnitude smaller than that of the liquid phase, the solid phase solute diffusion is ignored, and only the diffusion of the solute in the liquid phase and the interface cell is considered.

The solute diffusion model is based on Fick's first law, as in equation (4):

$$J = \frac{dm}{Adt} = -D_i \left( \frac{\partial C}{\partial x} \right)$$  \hspace{1cm} (4)

$J$ stands for solute diffusion flux; $D_i$ indicates solute diffusion coefficient, $i$ is cell state with two values: L and I (liquid and interface). $D_i$ can be calculated according to equation (5):

$$D_i = f_s D_s + f_l D_l$$  \hspace{1cm} (5)

$f_s, f_l$ represents solid fraction and liquid fraction; $D_s, D_l$ indicates the solute diffusion coefficient of solid and liquid, and it can be obtained according to the empirical formula, which take values $1 \times 10^{-3}$ and $1 \times 10^{-7}$ respectively in this paper.

Equation (6) is the solute transport equation established based on mass balance:

$$\frac{\partial C}{\partial t} \Delta x \Delta y \Delta t = J_{i-1,j} - J_{i+1,j} + J_{i,j-1} - J_{i,j+1}$$  \hspace{1cm} (6)

Interface solute redistribution follows local conservation:

$$C_i^* = C_l^*$$  \hspace{1cm} (7)

The equilibrium solute concentration in the interface can be calculated by equation (8) [22]:

$$C_l^* = C_0 + \frac{T^* - T_{l}^0}{m_l} + \frac{\Gamma K}{m_l}$$  \hspace{1cm} (8)

$C_0, T^*, T_{l}^0, K, \Gamma$ and $m_l$ indicates initial solute concentration, interface temperature, initial liquidus temperature coefficient, interface curvature and liquidus slope, respectively.

3. Numerical methods
3.1. Solution of the solute field

When the solid fraction of the cell increases by $\Delta f_s$, the amount of excess solute can be obtained by equation (9), which is derived from equation (7).

\[ dC = (1 - k) C'_i \Delta f_s \]  

(9)

If the remaining liquid of the current cell can completely receive the excess solute, the excess solute will be completely discharged to the remaining liquid, and the compositions of liquid and solid are updated by the equations (10) and (11), where $N$ represents the number of steps iterated from the start of solidification.

\[ C_{s,i}^{*+\Delta t} = \frac{C'_i \left(1 - f'_s\right) - kC'_i \Delta f'_s}{1 - f'_s} \]  

(10)

\[ C'_{s} = \sum_{n=1}^{N} k\Delta f'_s(n) C'_i(n) \]  

(11)

Otherwise: when $C_{s,i}^{*+\Delta t} > C'_i$, let $C_{s,i}^{*+\Delta t} = C'_i$ and $dC' = (C'_i - C_{s,i}^{*+\Delta t})\Delta f'_s$; if $f'_s = 1$, then $C_{s,i}^{*+\Delta t} = 0$ and $dC' = dC$.

While $dC' > 0$, if there are no liquid neighbours, $dC'$ will be enriched at the grain boundaries to form grain boundary segregation; otherwise, they will be reasonably distributed into the liquid neighbours. As shown in figure 1, in the case of the solute distribution is isotropic, $dC'$ will be evenly distributed in the circle, resulting in a difference in the amount of solute between the nearest neighbour and the next nearest neighbour, which can be represented by $\Delta C^n : \Delta C^{nn} = S^n : S^{nn} = 1: 0.52$. $S^n$ and $S^{nn}$ are the area of the nearest neighbour and the next nearest neighbour in the circle.

![Figure 1](image-url)  

**Figure 1.** Solute distribution diagram (interface cell, liquid cell).

Solute diffusion in liquid and interface is solved by cellular automaton method.

3.2. Growth and capture algorithms

As shown in figure 2, the shape of the grain is represented by an eccentric square, $\theta$ indicates its preferred orientation, the half-diagonal length is calculated by the equation (12):

\[ L(t) = \int_{t_0}^{t} v(\Delta T(\tau)) \, d\tau \]  

(12)

$v$ is the growth speed of the dendrite tip.
Figure 2. Dendrite evolution process in present model.

When the four vertices of the eccentric square contact the nearest neighbours \( B \) as shown in figure 2(b), \( B \) can be captured as the interface cell, so as \( C \) in figure 2(d).

All the captured cells inherit the growth parameters of \( A \). When all neighbours are captured, cell \( A \) is completely solidified. Solid fraction of the interface cell at time \( t \) can be calculated by equation (13):

\[
f_s(t) = S(t)/A
\]  

(13)

\( S(t) \) represents the solidified area of the cell.

4. Results and discussion

Figure 3 displays the evolution of dendrites simulated by the present model, which exhibits a clear dendritic morphology as well as secondary and high-order dendrites. (a), (b) and (c) correspond to the morphology of dendrites at time \( t_a = 0.2s \), \( t_b = 0.6s \) and \( t_c = 0.66s \), respectively.

The result of the model without considering the solute field is shown in figure 4. It can only simulate the outline of dendrite growth, and cannot fine dendritic structure. (a), (b), and (c) correspond to the morphology of dendrites at time \( t_a = 0.1s \), \( t_b = 0.3s \) and \( t_c = 0.34s \), respectively.

It can be seen from the figure 3(a) that the nucleated crystal first grows along the primary dendrite arm. As the solidification continues, the dendrites continuously extend into the melt, and the solute is enriched at the interface front; the interface of the dendritic arm loses equilibrium under the action of solute diffusion and surface tension, then the secondary dendrite arm shown in figure 3(b) is generated. Solute will also be enriched between the secondary dendrite arms, breaking the balance of the secondary dendrite arm interface, forming tertiary dendritic arms. And there will be more high-order dendritic arms before the end of solidification, eventually forming a dendritic crystal. If the influence of the solute field is neglected, as shown in the figure 4, the dendritic interface always advances steadily and maintains the state of the flat interface, so no branching is formed and the actual dendritic morphology cannot be simulated.
Figure 4. Dendrite evolution process in previous model.

In addition, the model can also simulate the distribution of solute in the interior of the dendrite and the front of the interface. Figure 5 shows the distribution of solute corresponding to the morphology of the dendrites in figure 3. It can be seen that the solute is enriched at the interface and it is not uniform inside the dendrite.

Figure 5. Solute distribution near dendrites.

The distribution of solute along the direction of the primary dendrites is shown in figure 6.

Figure 6. Solute distribution of primary dendrite arms.

The amplitude of the fluctuation between the two peaks of the curve represents the degree of segregation of the solute in the dendrites. The peaks on both sides represent the enrichment of the solute at the interface front. From figure 6, the distribution of the solute inside and at the front of the dendrite can be seen more clearly.
5. Conclusion
The present work improved the cellular automaton model and proposed a new solute distribution scheme, eventually completed the dynamic display of the dendrite evolution. Compared with the traditional model:

- The model can simulate the secondary and higher dendritic arms of dendrites;
- It is able to simulate the distribution of solute inside the dendrite and at the front of the interface.

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