Phase-field numerical simulation of three-dimensional competitive growth of dendrites in a binary alloy

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Abstract: The normal vector of migration direction in the solid-liquid interface of dendrites was used to describe the phase-field governing equation. By using the three angles formed by the normal vector for the migration direction of the dendritic growth interface and the coordinate axes of the simulation region, the authors expressed the interfacial anisotropy equation, and built a phase-field model for the competitive growth of multiple grains. Taking a Al-2% mole-Cu binary alloy as an example, the competitive growth of multiple grains during isothermal solidification was simulated by applying parallel computing techniques. In addition, the phase field simulation results were verified by the experimental method. The simulation results show that the competitive growth of equiaxed dendrite is divided into two types: the first occurs during the process of competitive growth, the tips of primary dendrite on different grains taking part in the competition stop growing in their optimal growth direction; the second also occurs during competitive growth, the tips of primary dendrite which participate in the competition on different grains never stop growing in their optimal growth direction. The dendritic morphologies of the first competition growth type are divided into two types. Primary dendrites of grains taking part in the competition stop growing in their optimal growth direction and the competition plane enlarges when neither one wins the competition. However, when one wins the competition, the primary dendrites of grains with superiority go through the blocking grains and continue to grow in their optimal growth direction. The primary dendrites of inferior grains stop growing in their optimal growth direction and then instead grow in those areas without obstacles. The dendritic morphology of the second competition-growth type is shown to be the deformation of primary dendrites, which are mainly represented as the deflection and bending observed from different views. Compared with the metallographic picture, the simulation results can show the morphology of the competitive growth in all directions, so this simulation method can better characterize the competitive growth process.

Key words: dendrite; Al-Cu binary alloy; competitive growth; dendritic morphology

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As an important simulation method, the phase-field method (PFM), which enables researchers to directly simulate the formation of microstructures, is an efficient tool for studying the structure of complex solidification interfaces. PFM can couple nucleation and growth models and influencing factors of nucleation and growth process with the basic heat transfer equation to carry out accurate microscopic numerical simulation. In

this way, the quantitative relationship of the effect of primary process parameters on the microstructure during material forming processes can be obtained. As an open model, the phase-field model can be coupled with various external fields such as temperature, dissolution, gravity, and fluid fields, and can effectively combine the microscale with the macroscale. With the development of the phase-field model and improvements in computing technology, quantitatively simulating and predicting the microstructure in the phase transition of actual materials by using PFM has become the focus of research into this aspect of material structures^[1-8].

Dendrite is a common solidification microstructure.

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During the past decade, simulations of dendritic growth by using PFM have become well developed. Simulation studies including 2-D^[9-18] and 3-D dendritic growth^[2,19-27], dendritic growth of pure substances^[9-11,19-20], dendritic growth in binary alloys^[1,12-15,21-25], and dendritic growth in multiple alloys^[2,16-18,26-27] have been reported. Multiple dendrites simultaneously grow during the casting process and their growth process can be directly simulated by using PFM^[1,28-31]. Mutual interactions and competitions exist among grains in the simultaneous growth of multiple grains. However, few studies have been carried out on the competitive growth among dendrites. Souhar and De Felice et al.^[32] simulated the mutual influence and competition of multiple 3-D dendrites simultaneously growing in a binary alloy by employing a mesoscopic model for solidification. Compared with PFM, mesoscopic models can readily simulate the mutual influence and competitive growth of 3-D dendrites due to the simplicity of calculation. However, although it entails simple calculations, it loses numerous detailed facets in the data. Takaki and Ohno et al.^[33,34] simulated competition growth and the mutual influence of 2-D dendrites in a binary alloy under directional solidification by applying PFM and a parallel numerical computation method. Turret et al.^[35] studied competitive growth of 2-D dendrites in a binary alloy during directional solidification by adopting PFM. Moreover, compared with the experimental data, they considered that the 3-D dendritic morphology plays an important role in dendritic orientation selection.

In this paper, by using PFM and parallel computing techniques, the 3-D competitive growth of multiple dendrites was simulated to reproduce the competitive growth of equiaxed dendrites in different directions. In addition, trends in competitive growth of dendrites were explored, as well as the morphological characteristics of competitive growth of dendrites and the effects thereof on dendritic orientation selection. Furthermore, the phase field simulation results were verified by the experimental method.

1 Phase-field model of competitive growth of dendrites

1.1 Phase-field and solute-field governing equations

Here, the normal vector in the solid-liquid interface of dendrites in migration direction is defined as follows:

$$\vec{n} = \frac{\nabla \phi}{|\nabla \phi|} \quad (1)$$

The phase-field governing equation described in the literature^[36] is employed:

$$\frac{\partial \phi}{\partial t} = M(\varepsilon(\theta)^2 \nabla^2 \phi + (\varepsilon(\theta) \cdot \varepsilon''(\theta) + \varepsilon'(\theta)^2) \cdot (|\nabla \phi| \nabla \vec{n}) - f_\phi) \quad (2)$$

where ϕ , M , and t represent the order parameter of phase field, the migration rate of solid-phase interface, and the time variable, respectively. Moreover, $\varepsilon(\theta)$ and f_ϕ refer to the parameter related to the surface energy and the first-order derivative of free energy density with respect to the order parameter of the phase field, respectively. The latter can be expressed as follows:

$$f_\phi = \frac{RT}{V_m} h'(\phi) \ln \frac{(1-c_s^e)(1-c_L)}{(1-c_L^e)(1-c_s)} + Wg'(\phi) \quad (3)$$

where R , T , V_m , $h(\phi)$, W , $g(\phi)$, and c represent the universal gas constant, temperature, molar volume, potential function, phase-field parameter, residual free energy function, and solute concentration of the alloy, respectively. Moreover, subscripts L and S as well as superscript e refer to the liquid phase, solid phase, and an equilibrium state, respectively.

The governing equation describing the diffusion and redistribution of solute can be written as follows:

$$\frac{\partial c}{\partial t} = \nabla \cdot \left(\frac{D(\phi)}{f_{cc}} \nabla f_c \right) \quad (4)$$

where $D(\phi)$ is the solute diffusion rate while f_c and f_{cc} represent the first- and second-order derivatives of free energy with respect to concentration, respectively.

1.2 Function equation for anisotropy of interfacial energy

There are three angles (θ_1 , θ_2 , and θ_3 , respectively) between the normal direction for the migration direction of the dendritic growth interface and the coordinate system:

$$\theta_1 = \arccos \left(\frac{\phi_x}{\sqrt{(\phi_x)^2 + (\phi_y)^2 + (\phi_z)^2}} \right) \quad (5)$$

$$\theta_2 = \arccos \left(\frac{\phi_y}{\sqrt{(\phi_x)^2 + (\phi_y)^2 + (\phi_z)^2}} \right) \quad (6)$$

$$\theta_3 = \arccos \left(\frac{\phi_z}{\sqrt{(\phi_x)^2 + (\phi_y)^2 + (\phi_z)^2}} \right) \quad (7)$$

where subscripts x , y , and z represent the first-order derivatives of the order parameter of the phase field with respect to the spatial coordinates x , y , and z , respectively. The angle θ between the normal direction for the migration of the dendritic growth interface and the optimal growth direction can be described by θ_1 , θ_2 , and θ_3 . Also, by using the θ as described by the three angles, the function for the anisotropy of interfacial free energy is defined^[36]. By using θ_1 , θ_2 , and θ_3 to define the equation for the anisotropy of interfacial energy, the following equation for the anisotropy of interfacial energy can be obtained:

$$\varepsilon(\theta) = 1 - 3\varepsilon_4 + 4\varepsilon_4(\cos^4 \theta_1 + \cos^4 \theta_2 + \cos^4 \theta_3) \quad (8)$$

In this model, θ_1 , θ_2 , and θ_3 need to meet the following requirement:

$$\cos^2 \theta_1 + \cos^2 \theta_2 + \cos^2 \theta_3 = 1 \quad (9)$$

Equations (8) and (9) control the growth orientation of grains, so the growth orientation of grains changes as the initial values of θ_1 , θ_2 , and θ_3 vary.

2 Phase-field parameters and numerical calculation of model

2.1 Determination of phase-field parameters

Migration rate M of solid-phase interface can be written as:

$$M^{-1} = \frac{\varepsilon_0^3}{\sigma \sqrt{2W}} \left(\frac{1}{D} \zeta (c_L^e, c_S^e) \right) \quad (10)$$

where ε_0 and W are phase-field parameters, which are calculated based on interface energy σ and interface thickness λ . They can be written as:

$$\varepsilon_0 = \sqrt{\frac{6\lambda\sigma}{2.2}} \quad (11)$$

$$W = \frac{6.6\sigma}{\lambda} \quad (12)$$

ζ is the interface migration parameter matrix. The expression can be written as:

$$\zeta = \frac{RT}{V_m} (c_L^e - c_S^e)^2 \times \int_0^1 \frac{h(\phi) [1 - h(\phi)]}{[1 - h(\phi)] c_L^e (1 - c_L^e) + h(\phi) c_S^e (1 - c_S^e)} \cdot \frac{d\phi}{\phi(1 - \phi)} \quad (13)$$

2.2 Material physical parameters

In this work, Al-2% mole Cu alloy was used to simulate dendritic growth. The physical parameters of the alloy are listed in Table 1.

Table 1: Material physical parameters

Physical parameters	Al-2% mole Cu
Interfacial energy σ , (J·m ⁻¹)	0.093
Melting temperature T_m , (K)	933.3
Equilibrium constant k^e	0.14
Diffusion coefficient of liquid-phase solute D_L , (m ² ·s ⁻¹)	3.0×10^{-9}
Diffusion coefficient of solid-phase solute D_S , (m ² ·s ⁻¹)	3.0×10^{-13}
Liquidus slope m^e , (K·mol ⁻¹)	620
Molar volume V_m , (m ³ ·mol ⁻¹)	1.0547×10^{-5}

2.3 Numerical calculation

The model was calculated using an MPI (message passing interface). Corresponding to the x -, y -, and z -axes of the rectangular coordinate system, the computational domain of the phase and solute fields was within an area of $400 \times 400 \times 400$ meshes, with a mesh size of 1×10^{-8} m ($\Delta x = 1 \times 10^{-8}$ m).

The initial nucleation was set as a sphere with the radius of the mesh being $R = 1 \times 10^{-7}$ m. By employing an explicit finite

difference method, equations (2) and (4) are synchronously solved with the same time-step Δt . Δt and space-step Δx ($\Delta x = \Delta y = \Delta z$) need to satisfy the following stable condition:

$$\Delta t < \min \{ \Delta x^2 / (6D_L), \Delta y^2 / (6D_L), \Delta z^2 / (6D_L) \} \quad (14)$$

The growth orientation of grains can be controlled by equation (8) and initial values of θ_1 , θ_2 , and θ_3 .

3 Results and analysis

3.1 Simulation results: morphology of competitive growth of multiple grains and concentrations of solutes

Figure 1 shows the simulation result for the competitive growth of four grains within the $400 \times 400 \times 400$ mesh. Figures 1 (a1-a6) show 3-D simulation results at various times, and the coordinate axes are included in the upper part of each figure. Figures 1(a1-a2), 1(a3-a4), and 1(a5-a6) show the simulation results at $600\Delta t$, $1,000\Delta t$, and $2,800\Delta t$, respectively. Figures 1(b1-b2) and 1(c1-c2) show the projections of the section in Fig. 1(a2) on the xoz -plane while the coordinates in Figs. 1(b1-b2) indicate the coordinate plane of Figs. 1(b1-b2) and 1(c1-c2). Figures 1(b3-b4) and 1(c3-c4) are projections of the section in Fig. 1(a4) on the $yo z$ -plane while the coordinates in Figs. 1(b3-b4) represent the coordinate planes of Figs. 1(b3-b4) and 1(c3-c4). Figures 1(b5-b7) and 1(c5-c7) are the projections of the section in Fig. 1(a6) on the $yo z$ -plane while the coordinates in Figs. 1(b5-b7) indicate the coordinate planes of Figs. 1(b5-b7) and 1(c5-c7). Figures 1(b1-b7) show the phase-field distribution of sections in the corresponding spaces while Figs. 1(c1-c7) indicate the distribution of the solute field of sections in the corresponding spaces. The upper colour scales in Fig. 1 show the order parameter of the phase field in the corresponding Figs. 1(b1-b7), while the bottom colour scales represent the scales of the solute content in the corresponding Figs. 1(c1-c7).

At $600\Delta t$, the four grains separately grow and reflect their own anisotropy on the interface without mutual interaction, as shown in Figs. 1(a1-a2), 1(b1-b2), and 1(c1-c2). At $1,000\Delta t$, two grains begin to touch each other while the other two do not begin to affect each other, as shown in Figs. 1(a3-a4), 1(b3-b4), and 1(c3-c4). At $2,800\Delta t$, the four grains show competition for growth to form a complex grain boundary, as illustrated in Figs. 1(a5-a6), 1(b5-b7), and 1(c5-c7). During the growth process, alloy grains release solute atoms which exert an effect on the distribution of the solute of surrounding liquid alloys, as shown in Figs. 1(c1-c7). The area between the two grains is mutually affected by the solute atoms released by the surrounding two grains, and, therefore, shows a high solute concentration, as shown in Figs. 1(c5-c7). According to the colour scale of solutes shown in the figure, the roots of primary branches of the dendrites also exhibit high solute concentrations. In the liquid metal area affected by multiple grains, the competitive growth of grains changes the morphology of the dendrites to form the grain boundaries with complex structures because of mutual competitive growth of grains.

Fig. 1: Simulation results and sectional drawings at different times in competitive growth of multiple grains

To observe the morphologies of each grain competition for growth and to summarise the trends influencing competitive growth on the morphology of the grains, Figure 2 shows the morphologies of all grains corresponding to Fig. 1(a5). Figure 2(a1) shows a 3-D image of Fig. 1(a5) observed from the view of the xyz - o plane and the relevant view coordinates are shown as the coordinates in the top left-hand corner of Fig. 2. Figures 2(a2-a5) show 3-D images of the four grains observed from the same view. Figures 2(b1-b5) show Figs. 2(a1-a5) on the yox -plane while Figs. 2(c1-c5) show Figs. 2(a1-a5) on the zox -plane. Moreover, Figures 2(d1-d5) show Figs. 2(a1-a5) on the zoy -plane. In Fig. 2, the grains in Fig. 2(a2) make contact

with those in Fig. 2(a4) and their preferred growth orientations are similar. Therefore, the grain boundaries between them can be classified as low-angle boundaries. However, the grains in Fig. 2(a3) make contact with those in Fig. 2(a5) showing a significant difference in preferred growth orientations, so the grain boundaries between them can be classified as high-angle boundaries. In addition, at $2,800\Delta t$, no grain boundary was seen between each pair of contacting grains. As can be seen from Fig. 2, although non-contacting dendrites have no crystal boundary, they still influence each other, which causes deformation of the grain morphology, e.g., the deformation of the upper-, and right-branches of the grains shown in Fig. 2(b2).

Fig. 2: Simulation of morphologies during competitive growth of multiple grains and single grains (different views)

3.2 Analysis and discussion of competitive growth of multiple grains

According to the simulation results, the mutual influence among grains produced during competitive growth of multiple grains can be divided into two types: (1) during the competitive growth, the tips of the primary branches of those dendrites participating in the competition on different grains stop growing in their optimal growth direction; (2) during competitive growth, the tips of the primary branches of the dendrites taking part in the competition do not stop growing in their optimal growth direction.

In Figs. 2(a2) and (a4), the competition of grains belongs to the first type: at $600\Delta t$, the upper primary branch of the grain in Fig. 2(a2) has no contact with any other or the lower primary branch of the grain in Fig. 2(a4), as shown in Figs. 1(a1–a2) and 1(b1–b2). In time, the tips present increasingly narrow separations and finally make contact with each other, as shown in Figs. 1(a3) and 1(b4). Finally, the primary branches of the two dendrites stop growing in the direction (parallel to the z -axis) after making contact, as shown in Figs. 1(b7) and 2(c1). The competitive growth of grains in Figs. 2(a3) and 2(a5) also belongs to this type, but it displays certain differences therewith. The optimal growth direction of the primary dendrites of grains in Figs. 2(a2) and 2(a4) was at a low angle, while those in Figs. 2(a3) and 2(a5) grow at a steeper angle. The details of their differences are described below.

The competition of grains in Figs. 2(a3) and 2(a4) is of the second type, as shown in Figs. 2(b1), 2(b3), and 2(b4). The lower primary branch of the grain in Fig. 2(b3) interacts with

the right primary branch of the grain in Fig. 2(b4), resulting in a morphological deformation of the primary branches. Competition between grains in Figs. 2(a3) and 2(a4) also belongs to this type, as shown in Figs. 2(d1), 2(d3), and 2(d5). The morphology of the primary branch of the grain pointing outward (parallel to the x -axis) in Figs. 2(d2) and 2(d4) deflects. The deflection is performed as the deformation of the right primary branch of the grain seen in Figs. 2 (b2) and 2 (b4) from the perspective of the x -axis.

As mentioned above, in the competitive growth of the first type, different grains having large or small angles between their optimal growth directions show different morphologies. Figure 3 shows the morphologies of dendrites competing for growth forming a large angle with the optimal growth directions. Figures 3(a1–a5) show the morphologies of the two grains observed from different views and the coordinate axes above the figures correspond to the direction of the view. Figures 3(b1–b5) display the morphologies of one grain winning the competition observed from different views and the coordinate axes above the figures correspond to the direction of the view. Figures 3(c1–c5) show the morphologies of the grain losing the competition from different views. The competition result of the two grains is shown in the lower area of Fig. 3(a2) where the two grains make contact. The primary branches of the winning grain in the competition go through the blocking grain and continue to grow in its direction of optimal growth, as the bottom primary branch shown in Fig. 3(b2). In comparison, the primary branches of the inferior grain stop growing in the optimal growth direction and then turn to grow in areas without obstacles, as shown in Figs.

Fig. 3: Simulated morphologies of two grains with high-angle boundaries in competitive growth

3(a2) and 3(c2). For different grains with small angles between the optimal growth directions of such dendrites, competitive growth between dendrites in Figs. 2(a2) and 2(a4) is not observed.

Classic theory suggests that the section of a dendrite tip is parabolic upon isothermal solidification^[37,38]. Ivantsov derived an equation for calculating the dendrite tip velocity and constructing the shape curve of the dendrite tip^[39]. By observing the grain morphologies in Figs. 1(b7) and 3, it can be seen that morphologies of the primary branches not participating in competitive growth conform to classical theory. Morphologies of the primary branches of grains taking part in the competition present different morphological features for the two types of competitive growth mentioned earlier.

The dendritic morphology of the first type of competitive growth shows the following features: a plane is formed between the dendrite tip and the competitive dendrite which prevents its normal growth in the area under competition. Both dendrites in the competition stop growing in the direction perpendicular to this plane, while they begin to compete for growth in the direction parallel to this plane. The primary branches of the grains which take part in the competition stop growing in their optimal growth directions when the optimal growth directions form a small angle. As a result, the competition plane enlarges, namely, neither one wins the competition, which can be observed from the competitive growth of grains in Figs. 2(a2) and 2(a4). When the optimal growth directions of the primary branches of grains taking part in the competition form a large angle with the optimal direction, the primary branches stop growing before one wins the competition. Also, the competition plane extends [see the competitive growth of grains in Figs. 2(a3) and 2(a5)]. When the competitive primary branches of the grains form a large angle with the optimal growth direction and win the competition, the primary branches of the superior grain cross the blocking grain and continue to grow in their optimal growth direction. The primary branches of the inferior grain stop growing in the optimal growth direction and then turn to grow in areas without obstacles, as shown in Figs. 3(b3) and 3(c5).

The dendritic morphology of second type of competitive growth shows the following features: the morphology of primary branches of different grains is deformed due to the influence of the primary branches of the competing grains. The deformation is expressed as a deflection or bending as observed from different views.

3.3 Experimental results

The Al-2%molCu binary alloy was melted in an intermediate frequency induction furnace, and the sample was prepared by metal mold casting. Metallographic images are shown in Fig 4.

In Fig. 4, the competitive growths between grains A and B and grains F and G include two cases of the first type of competitive growth, as described above, which are the competitive growth of grains in Fig. 1(b7) (two-dimensional plane) and Figs. 2(a2) and 2(a4) (three-dimensional morphology), the competitive growth of grains in Fig. 1(b5) (two-dimensional plane) and Figs. 2(a3) and 2(a5) (three-dimensional morphology), respectively. The competitive growths between grains C and D, and grains C and E, belong to the second type of competitive growth, as described above in Figs. 2(a3) and 2(a4) (three-dimensional morphology).

Through the metallographic picture, the morphology of the competitive growth can be seen, but it is a two-dimensional plane which is just seen from a single direction, while the simulation method can show the morphology of the competitive growth in all directions. Therefore, the simulation method can better characterize the competitive growth process.

4 Conclusions

(1) The 3-D competitive growth of multiple dendrites is simulated to reproduce the competitive growth of equiaxed dendrites in different directions using PFM and MPI parallel computing. The competitive growth of multiple grains found in the simulations agreed well with the experimental results.

(2) The competitive growth of equiaxed dendrites can be divided into two types: the first one, the tips of competitive primary branches of different dendrites stop growing in their optimal growth direction; and the second one, the tips of competitive primary branches of different dendrites do not stop growing in their optimal growth direction during competitive growth.

(3) The morphology of the dendrites during their growth displays the following characteristics: the dendrites showing the first type of competitive growth can be divided into two cases. The competitive primary branches of dendrites stop growing in their optimal growth direction and the competitive growth plane enlarges when neither one wins the competition. The primary branches of the dendrite winning the competition cross the blocking one and continue to grow in the direction of

Fig. 4: Microstructure of Al-2%molCu binary alloy

optimal growth. The primary branches of the dendrite losing the competition stop growing in their optimal growth direction and then they turn to grow in areas without obstacles. The morphology of primary branches of the dendrite in the second type of competition is deformed through deflection and bending as observed from different views.

(4) Compared with the metallographic picture, the simulation results can show the morphology of the competitive growth in all directions, so the simulation method can better characterize the competitive growth process.

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