

Phase field modeling of dendritic coarsening during isothermal solidification

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Abstract: Dendritic coarsening in Al-2mol%Si alloy during isothermal solidification at 880K was investigated by phase field modeling. Three coarsening mechanisms operate in the alloy: (a) melting of small dendrite arms; (b) coalescence of dendrites near the tips leading to the entrapment of liquid droplets; (c) smoothing of dendrites. Dendrite melting is found to be dominant in the stage of dendritic growth, whereas coalescence of dendrites and smoothing of dendrites are dominant during isothermal holding. The simulated results provide a better understanding of dendrite coarsening during isothermal solidification.

Key words: phase field; dendritic coarsening; Al-Si alloy; isothermal solidification

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Phase field models are known to be very powerful in describing the complex pattern evolution of dendritic growth. It is a useful method for realistically simulating microstructure evolution involving diffusion, coarsening of dendrites and the curvature and kinetic effects on the moving solid-liquid interface. Such models are efficient, especially in numerical treatment, because all the governing equations are written as unified equations in the whole space of the system without distinguishing the interface from the mother and the new phase, and direct tracking of the interface position is not needed during numerical calculation. In the last decade, the phase field method has been intensively studied as a model of solidification processes^[1-5]. The coarsening behavior affects the distribution of length scales, micro-segregation and other microstructural characteristics of the materials, all of which determine the physical and chemical properties of materials in terms of strength, ductility and corrosion resistance. Therefore, understanding coarsening and being able to study the morphology of the dendritic structure are of technological importance^[6-8]. Many properties of cast materials are intimately related to the dendritic morphology that is largely set by coarsening. Even if the effect of the dendritic microstructure is altered by subsequent heat treatment, these properties rarely fully disappear.

In this paper, the dendritic growth and the subsequent dendritic coarsening in Al-2mol%Si alloy during isothermal solidification at 880K were simulated using a phase field model. The simulation results show three coarsening mechanisms in the alloy.

1 Phase field model

The phase field model includes two variables: one is a phase field $\phi(x,y,t)$ and the other is a concentration field $c(x,y,t)$. The variable $\phi(x,y,t)$ is an ordering parameter at the position (x,y) and the time t , $\phi = 1$ means being solid and $\phi = 0$ liquid. The solid-liquid interface is expressed by the steep layer of ϕ connecting the value 0 and 1. So the phase field model can be described^[9-10] as:

$$\frac{\partial \phi}{\partial t} = M(\varepsilon^2(\theta)\nabla^2\phi - f_\phi) \quad (1)$$

$$\frac{\partial c}{\partial t} = \nabla \cdot \left(\frac{D(\phi)}{f_{cc}} \nabla f_c \right) \quad (2)$$

where, $f(c, \phi) = h(\phi)f^S(c_S) + (1-h(\phi))f^L(c_L) + Wg(\phi)$ (3)

$$D(\phi) = D_L + h(\phi)(D_S - D_L) \quad (4)$$

$$h(\phi) = \phi^3(6\phi^2 - 15\phi + 10) \quad (5)$$

$$g(\phi) = \phi^2(1 - \phi^2) \quad (6)$$

$$c = h(\phi)c_S + (1-h(\phi))c_L \quad (7)$$

$$\mu^S(c_S(x,t)) = \mu^L(c_L(x,t)) \quad (8)$$

$$f^S = c_S f_B^S(T) + (1-c_S) f_A^S(T) \quad (9)$$

$$f^L = c_L f_B^L(T) + (1-c_L) f_A^L(T) \quad (10)$$

$$\varepsilon(\theta) = \varepsilon_0(1 + v \cos k\theta) \quad (11)$$

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$$M^{-1} = \frac{\varepsilon^2}{\sigma} \left[\frac{RT}{V_m} \frac{1-k^e}{m^e} \frac{1}{\mu} + \frac{\varepsilon}{D_L \sqrt{2W}} \zeta(c_S^e, c_L^e) \right] \quad (12)$$

$$\zeta(c_S^e, c_L^e) = f_{cc}(c_S^e) f_{cc}^L(c_L^e) (c_L^e - c_S^e) \times \int_0^1 \frac{h(\phi_0) [1-h(\phi_0)] d\phi}{[1-h(\phi_0)] f_{cc}^S(c_S^e) + h(\phi_0) f_{cc}^L(c_L^e) \phi_0 (1-\phi_0)} \quad (13)$$

$$\varepsilon = \sqrt{\frac{6\lambda}{2.2}} \sigma \quad (14)$$

$$W = \sqrt{\frac{6.6\sigma}{\lambda}} \quad (15)$$

where M and ε are the phase field mobility and gradient energy coefficient, respectively, and f is the free energy density of the system. The subscripts under f indicate the partial derivatives. $D(\phi)$ is the diffusivity of solute as a function of phase field. D_S and D_L are the diffusive coefficients in the solid and liquid, respectively; $h(\phi)$ and W correspond to the solid fraction and the height of double-well potential, respectively; c_L and c_S are the solute concentration in liquid and solid, respectively; ε_0 is the mean value of ε ; θ is the angle between the normal to the interface and the X-axis; $\theta = \arctan(\phi_y/\phi_x)$. v is the magnitude of anisotropy and k is the mode number, $k=4$. m^e is the equilibrium slope of the liquids; k^e is the equilibrium partition coefficient. The phase field parameters of ε and W are related to the interface energy σ and the interface width 2λ .

In addition, stochastic noise is introduced into the phase field equation to cause fluctuations at the solid/liquid interface that leads to the development of a dendrite structure. Herein, noise is introduced by modifying the phase field equation:

$$\frac{\partial \phi}{\partial t} \rightarrow \frac{\partial \phi}{\partial t} + 16g(\phi)\chi\omega \quad (16)$$

Where χ is a random number distributed uniformly between -1 and 1, and a new number is generated for every position of the grid at each time-step. ω is the amplitude of the fluctuations.

The two-dimensional simulation was performed at 880K in an Al-2mol%Si alloy with thermo-physical data given as: $\sigma = 0.093 \text{ J}\cdot\text{m}^{-1}$, $T_m = 922\text{K}$, $V_m = 1.06 \times 10^{-5} \text{ m}^3/\text{mol}$, $k^e = 0.0807$, $D_L = 3 \times 10^{-9} \text{ m}^2\cdot\text{s}^{-1}$, $D_S = 1 \times 10^{-12} \text{ m}^2\cdot\text{s}^{-1}$, $m^e = -939.0$, $v = 0.03$, and $\omega = 0.01$.

In the calculation, the governing equations were solved on uniform grids by using an explicit finite difference method. The two dimensional square calculation domains of 1,000 \times 1,000 grids for the phase field and solute field are prepared. The grid size of the phase field and the concentration field is $1 \times 10^{-8} \text{ m}$.

2 Results and discussion

Figure 1 illustrates the solid fraction as a function of solidification time in dendritic growth and dendritic coarsening for Al-2mol%Si alloy at 880K during isothermal solidification. The selected snapshots show the dendritic growth and coarsening, corresponding to the solid fraction and solidification time from "A" to "I" indicated in Fig. 1. With the solidification proceeding, the solid fraction is increased. The microstructure is evolved into a highly interconnected structure. When the solidification time is 0.36 ms, the primary dendrite tip just impinges on the boundary of the domain. At this time, the solid fraction is 27.6%, as shown in "A" position. Table 1 lists the variation of solid fraction with solidification time during isothermal solidification at 880K. When the solid fraction reaches 65.3%, the microstructural evolution

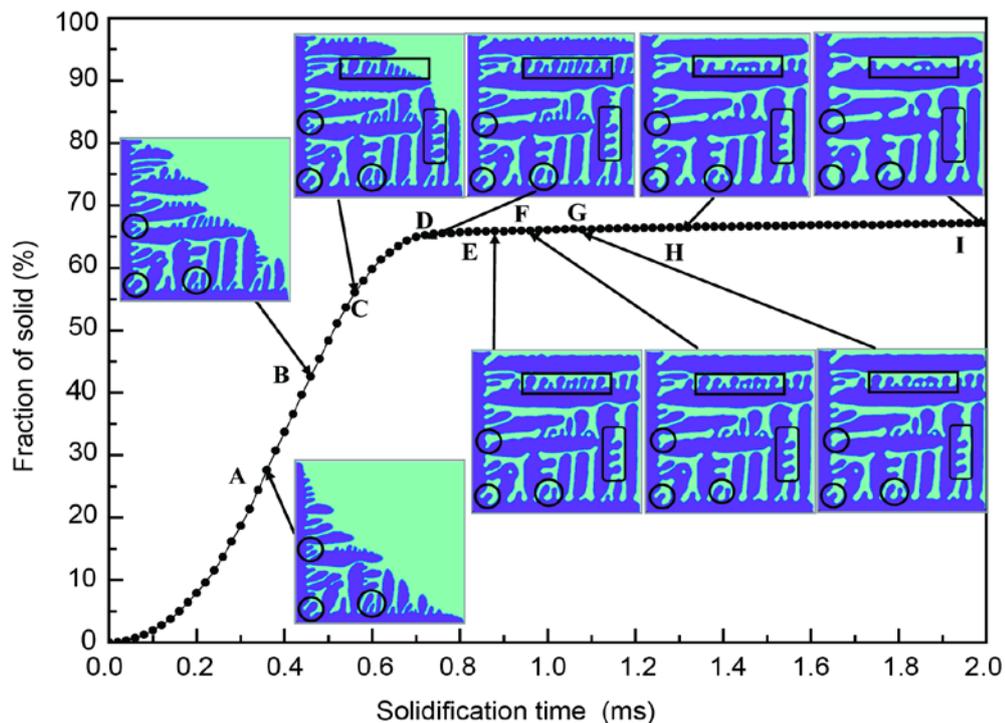


Fig. 1: The solid fraction as a function of solidification time for Al-2mol%Si alloy during isothermal solidification at 880K

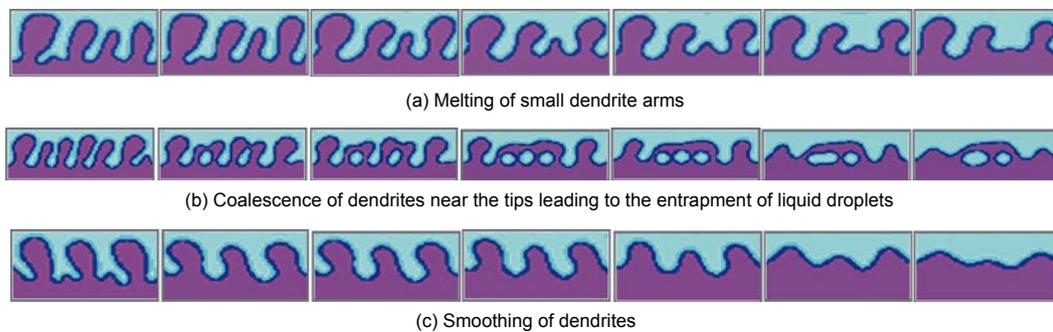
Table 1: The variation of solid fraction with solidification time at 880K during isothermal solidification

	Position								
	A	B	C	D	E	F	G	H	I
Solidification time (ms)	0.36	0.46	0.56	0.72	0.88	0.96	1.06	1.30	2.00
Solid fraction (%)	27.6	42.6	56.0	65.3	65.9	65.9	66.1	66.5	67.2

comes into the domination of dendritic coarsening. When the solid fraction is less than 65.3%, the growth of dendrite is dominant and the solid fraction increases rapidly. When the solid fraction is more than 65.3%, the dendritic coarsening is dominant and the solid fraction increases slowly. The dendritic coarsening is as the result of the competition of side branch growth. Dendrite melting is found to be dominant in the stage of dendritic growth, whereas coalescence of dendrites (as indicated in the rectangular areas in Fig. 1) and smoothing

of dendrites (as indicated in the round-cornered rectangular areas in Fig. 1) are dominant during isothermal holding. As we can see, dendrites with small size gradually melt away from their tips towards their roots and eventually disappeared (as indicated in the circled areas in Fig. 1).

Figure 2 shows the three coarsening mechanisms in Al-2mol%Si alloy during isothermal solidification at 880K. In the early stage, the dendrite arms including small arms and large arms keep growing. Dendrites with smaller tip size than their neighbors gradually melt from the tips towards the roots and axial melting is dominant. During isothermal holding, the dominant coarsening mechanism is coalescence and smoothing of dendrites. Three coarsening mechanisms operate in the alloy: (a) the melting of small dendrite arms; (b) the coalescence of dendrites near the tips leading to the entrapment of liquid droplets; and (c) the smoothing of dendrites.

**Fig. 2: The three coarsening mechanisms in Al-2mol%Si alloy at 880K during isothermal solidification**

3 Conclusions

The phase field method is a powerful tool not only in modeling of dendritic growth but also in dendritic coarsening. The dendritic growth and dendritic coarsening in Al-2mol%Si alloy during isothermal solidification at 880K were simulated using the phase field model.

With the solidification proceeding, the solid fraction is increased. The microstructure evolves into a highly interconnected structure. When the solid fraction reaches 65.3%, the microstructural evolution comes into the domination of dendritic coarsening. Dendrite melting is found to be dominant in the stage of dendritic growth, whereas the coarsening of dendrites is dominant during isothermal holding.

Dendrites with smaller tip size than their neighbors gradually melt from the tips towards the roots. Axial melting is dominant. Three coarsening mechanisms operate in Al-2mol%Si alloy during isothermal solidification at 880K, which are the melting of small dendrite arms, the coalescence of dendrites near the tips leading to the entrapment of liquid droplets, and the smoothing of dendrites.

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