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Influence of the Melt Flow Rate on Dendrite Micro Segregation During Alloy Solidification Simulated by Phase Field Method

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Abstract: The dendrite growth of binary alloy Al-Si under the forced convection was simulated by the phase field model coupled with the solute field and flow field. The influences of the forced convection on the morphology of the dendrite growth, the distribution, diffusion layer and micro-segregation of the solute, etc. were studied. The results show that the morphology of the dendrite growth, the distribution, diffusion layer and micro-segregation of the solute were significantly changed under forced convection. With increasing of the convection speed, the growth of the dendrite is asymmetric. The upstream dendrite growth rate is greater than that of the downstream. The secondary dendrite at upstream was more developed and the dendrite in normal direction was bias more serious to the upstream. In the upstream, the concentration gradient at dendrite tip frontier increases and the thickness of the solute diffusion layer decreases. On the contrary, the concentration gradient decreases in the downstream and the thickness of the solute diffusion layer increases. Furthermore, micro segregation of the dendrite also becomes more serious caused by the effect of convection. The simulation results are consistent with solidification theory.

Key words: Phase field method, forced convection, dendrites, micro segregation

INTRODUCTION

The dendrite is a common microstructure during the alloy solidification molding process, whose morphology and solute distribution determine the properties of the material. The growth of the dendrite is a complex physical processes comprehensively influenced by the various factors, such as heat and mass transfer, interface structure and dynamics, etc. During the solidification process, the solute and the temperature distribution of the liquid metal are strongly changed by the convection, which significant influences the dendrite growth process, the solute segregation, shrinkage porosity, shrinkage void and other defects distribution of the solidification structure. Therefore, it is of great significance to study on the role of the melt flow in the solidification process. The simulation of the dendrite growth coupled with flow field in the solidification process is becoming a research focus for the domestic and foreign scholars.

The phase field model coupled with the external temperature solute and flow field could realistically simulate the influence of the liquid metal convection on the solidification microstructure morphology and solute distribution, which currently attract wide attention domestic and foreign researchers. Based on the phase field model established by Karma, a new phase field model considered the flow field was proposed by Tong *et al.* (2000) and the influences of the flow rate, flow direction and anisotropy under forced convection on the dendritic morphology, the tip advancing speed as well as the morphology selection were firstly simulated (Tong *et al.*, 2001; Lu *et al.*, 2005). By simplifying the convection to the shear flow, the dendrite growth under the effect of the shear flow was simulated by using adaptive finite element method (Tonhardt and Amberg, 1998, 2000). It was found that found the dendrite growth in the upstream was promoted, while that in downstream was inhibited. The dendrite growth under the conditions of low supercooling and forced convection was simulated by using phase field method, realizing the large analog scale calculation under low supercooling condition (Lan *et al.*, 2002; Lan and Shin, 2004; Lan *et al.*, 2006). Jeong *et al.* (2001, 2003) simulated the influence of the melt flow on the three-dimensional dendritic growth by adaptive finite element method, which is quite different with that in two-dimensional. The reasons were analyzed. Recently, the dendtritic growth in the non-isothermal solidification of binary alloy has been studied with the constant temperature boundary conditions by Long *et al.* (2009).

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Up to now, the phase field simulation coupled with flow field mainly focused on the elementary substance. There is rare contribution devoted to the flow field for the alloy dendrite growth. In this study, based on phase-field model proposed by Kim and Tae Kim (2001) and coupled with solute field and flow field for numerical calculation, dendrite growth and the solute distribution of Al-3.0% Si binary alloy in the solidification process under flow field were simulated. The influences of the forced convection on the morphology of the dendrite growth, the distribution, diffusion layer and micro-segregation of the solute, etc., were studied.

MATHEMATICAL MODELS

Phase-field model: For the binary alloy system, the phase field governing equation is as follows Kim and Tae Kim (2001):

$$\frac{\partial\phi}{\partial t}=M\begin{bmatrix}\varepsilon^2\nabla^2\phi+\dfrac{RT}{V_m}h'(\phi)\ln\dfrac{(1-c_L).(1-c_S^e)}{(1-c_S).(1-c_L^e)}\\-Wg'(\phi)\end{bmatrix}\tag{1}$$

where, M the moving speed of the phase field related to the interface driving force; t time; R the gas constant; T temperature; V_m molar volume; ε, W phase field parameters; c the concentration of the solute; subscript S and L represent the solid and liquid phases, respectively; superscript e represents equilibrium; $h(\phi) = \phi^3\ (10\text{-}15\phi+6\phi^2)$ the potential function, $g(\phi) = \phi^3\ (1\text{-}\phi^2)$ the excess free energy function.

Solute diffusion equation: The solute field governing equation coupling with flow field is as follows:

$$\frac{\partial c}{\partial t}+\nabla\cdot(Vc)=\nabla\left[D(\phi)\nabla c+D(\phi)h'(\phi)(c_L-c_S)\nabla\phi\right]\tag{2}$$

where, $D(\phi) = D_L+h(\phi)\ \ (DS\text{-}D_L)$ the solute diffusion coefficient, D_S and D_L represent the solute diffusion coefficient in the solid phase and a liquid phase, respectively.

Mass and momentum conservation equations: In order to unified descript alloy melt flow in the liquid region and among the dendrite, it is assumed that the position of the dendrite was not changed under the convection during the solidification process. The melt flow velocity meets the mass conservation and Navier-Stokes equations. The equations coupling with the field equations are as follows:

$$\nabla.\ ((1\text{-}\phi)V) = 0\tag{3}$$

$$\frac{\partial V}{\partial t}+V\cdot\nabla\frac{V}{1-\phi}=-\frac{1-\phi}{\rho}\nabla P+\mu\nabla^2V-M_1^d\tag{4}$$

where, V the velocity vector; P the pressure; ρ the density. In this study, it is assumed that the density of solid phase was equal to that of the liquid phase and was a constant. ì the kinetic viscosity; $M_i^d = \mu h\phi^2 v/\varepsilon^2$ the attenuated interfacial phase resistance, h = 2.757.

NUMERICAL ISSUES

Numerical method: In this study, the phase field governing Eq. 1 and solute governing field Eq. 2 were synchronously solved by explicit finite difference method. The continuity Eq. 3 and the momentum Eq. 4 were solved by SIMPLE algorithm based on the collocated grid. The calculation time step was limited by the calculation of concentration field, i.e. $\Delta t<\Delta\times2/4DL$ and $\Delta t = \Delta\times2/5DL$ in the calculation process. According to the symmetry of the dendrite, only half of the dendrite growth area was calculated to save time. The number of computational grid was 700×350 and the mesh size was 1.0×10^{-8} m. The Al-3.0 mol% Si alloy was selected for study and the material parameters were shown in Table 1.

Initial and boundary conditions: For the beginning of the calculation process, it was assumed that the entire computational domain was filled with homogeneous supercooling alloy melt. The primary nucleation is set to triangle grids of 30×15. In this triangle area, the initial phase field variable values of the nodes in this region were 1, as the crystal nucleus. The other nodes were 0, related to the state of the supercooling liquid phase; the initial temperature was 882 K. An inlet velocity V_{in} was applied at the left edge of the simulation region and the fluid was transverse the right of the outflow boundary. The alloy melt flow velocity at the initial moment were set as $V_x = u_0$ and $V_y = 0$, the initial pressure p = 0, the initial value of concentration field 3.0 mol%. On the boundary of the computational domain, the Neumann boundary condition was selected for the phase and concentration fields.

Table 1: Material parameters of Al-3.0 mol% Si alloy

Material	σ (J m^{-2})	D_L (m^2 sec^{-1})	D_S (m^2 sec^{-1})	m_e (K mol^{-1})	k_e	Cp kJ kg^{-1} K^{-1}	μ (m^2 sec^{-1})
Al-Si	0.093	3.0×10^{-9}	3.0×10^{-13}	-682.0	0.0807	1.13	1.0×10^{-6}

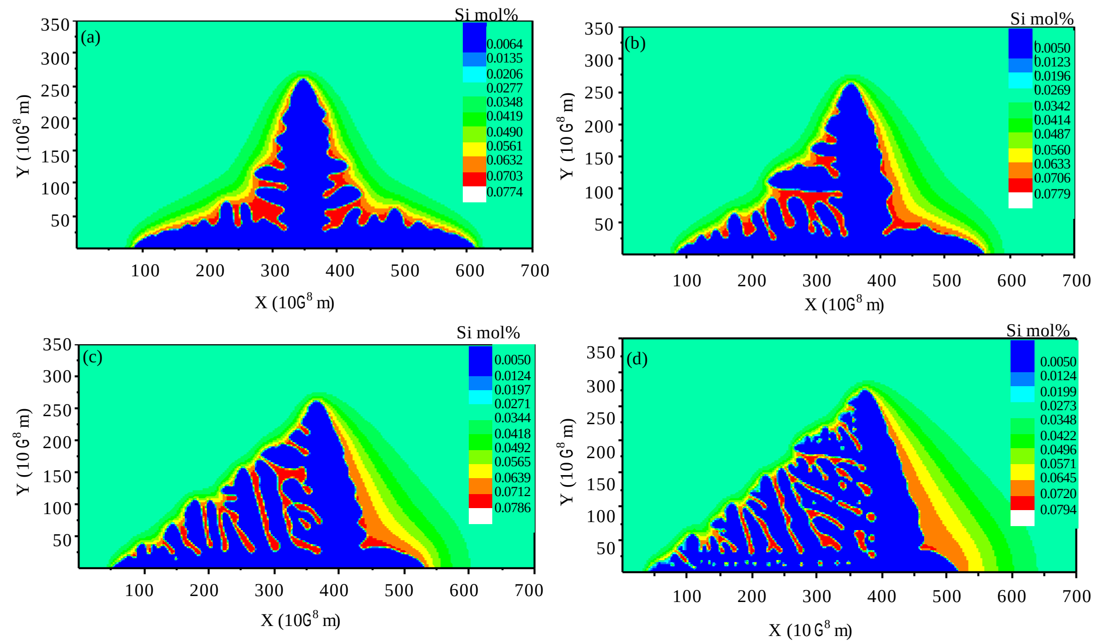

Fig. 1(a-d): Dendrite morphologies and solute field distributions at different flow rate, (a) v = 0.0 m sec^{-1}, (b) v = 0.01 m sec^{-1}, (c) v = 0.02 m sec^{-1} and (d) v = 0.03 m sec^{-1}

RESULTS AND DISCUSSION

Dendrite morphology and solute field: The morphologies of the Al-3.0 mol% Si alloy dendrites at the same moment under different flow velocities (v = 0.0, 0.01, 0.02, 0.03 m sec^{-1}) were shown in Fig. 1. It can be seen in Fig. 1 that the morphology of dendrite is symmetry with undeveloped secondary dendrite, when the convection velocity is zero. With the presence of convection, the symmetry of the dendrite morphology was destroyed. The main dendrite arm in normal direction was bias to the upstream and the dendrite at upstream was more developed with faster growth rate. The dendrite growth at downstream was inhibited. Moreover, the greater the convection velocity, the faster the upstream dendrite growth at the same time and the more developed the secondary dendrite. The triple dendrite generated when the flow rate was large. The dendrite growth at downstream was relative slow and there was rare secondary dendrite. The dendrite in normal direction was bias more serious to the upstream. This is mainly because the solute was flushed from the upstream to the downstream under the melt flow, leading to the lower concentration the in the upstream liquid phase. The liquidus slope of this alloy is negative. Under constant isothermal conditions with the same supercooling temperature, the lower the solute concentration, the smaller the constitutional supercooling. Therefore, the actual supercooling is greater and the growth rate of the upstream dendrite is greater than that of downstream, leading to the asymmetric dendrite growth morphology. Hence, the simulation results are consistent with the classical solidification theory.

The solute distribution of the Al-3.0 mol% Si alloy dendrites at the same moment under different flow velocities (v = 0.0, 0.01, 0.02, 0.03 m sec^{-1}) were shown in Fig. 1. During the solidification process, due to the supercooling caused by the curvature effect of dendritic tip, the solidus was moved down. The diffusion rate of the solute in solid phase is much lower than the dendrite growth rate, leading to the minimum Si concentration distributions at the center of the dendrite. The concentration distribution at the center of the dendrite under different flow velocities were shown in Fig. 2. It can be seen in Fig. 2 that with increasing of the flow velocity, the Si concentration of at the center of dendrite principal axis in the upstream becomes higher and higher, while that in the downstream is getting lower and lower, because the growth of upstream dendrite tip becomes faster with increasing of the melt flow velocity, leading to the smaller radius of curvature and smaller supercooling effect. As a result, the solidus moves down with smaller distance. For the downstream, the situation is on the contrary.

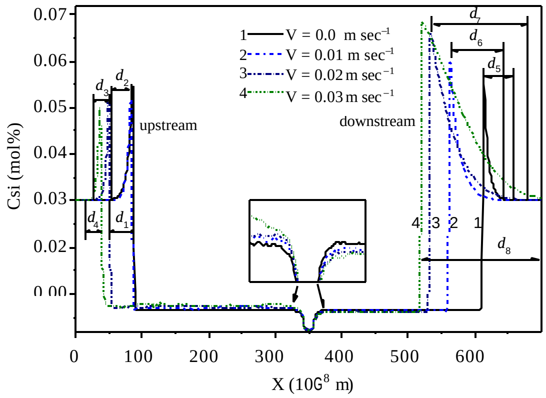

Fig. 2: Concentration distributions at the center of the dendrite

In the dendrite growth process, the element Si enriched in the solidification area because of the solute redistribution during the solidification process. The Si concentration in solid phase is lower than the initial concentration and the diffusion speed of the solute in the liquid phase is lower than the growth rate of the dendrite. Hence, the precipitated solute during the solidification process could not sufficiently diffuse into the liquid phase and thereby enriched in the forefront of the dendrite. The distribution of the solute field is symmetry without convection. When the melt flows, the solute distribution was dramatically changed with the variation of the dendrite morphology. Because of convection, the solute was scored from upstream to downstream, so that the solute concentration at solid-liquid interface in the upstream decreased, while that in the downstream increased. However, due to larger speed of the upstream dendrite growth and the well developed dendrite, the secondary or triple crystal arms generated between the primary dendrite arm, leading to the solute enrichment. As a result, the solute was difficult to diffuse into the liquid phase and solute concentration in the entire region was relatively high. The position of the highest solute concentration was usually in this region and the concentration increased with the increasing of the flow speed.

Solute diffusion layer at solid-liquid interface: According to the solute redistribution theory in the solidification process of single-phase alloy, there is a diffusion layer at the solid-liquid interface under condition of convection. It can be seen in Fig. 1 that a certain concentration gradient exists at the front of the dendrite solidification and the concentration gradient variation at dendrite tip cutting-edge is obvious under the different flow rates. This concentration gradient region is the solute diffusion layer. As the tip of the dendrite main arm grows fastest and there is not enough time for the solute to diffuse, the concentration gradient in this area is the largest and the solute diffusion layer is the smallest. As the root of the dendrite main arm grows slowest and the solute sufficiently diffused, the concentration gradient in this area is the smallest and the solute diffusion layer is the largest. When the flow velocity is zero, the solute fields at dendrite tip in both upstream and downstream symmetric distribute and the concentration gradients are nearly the same. With the enhancement of the convection, the equal concentration lines at the forefront of the upstream dendrite become more and more dense, the concentration gradient increases and the solute diffusion layer is reduced. On the contrary for the downstream, the equal concentration lines become fewer and fewer, the concentration gradient becomes smaller and smaller and the solute diffusion layer increases.

It could be more intuitively seen in Fig. 2 the variation regulation of the solute diffusion layer at forefront of the dendrite tip. Under the effect of convection, the solute diffusion layer at the upstream dendrite tip is smaller than that of the downstream. With increasing of the flow rate, the diffusion layer thickness in the upstream decreases while that in the downstream increases. The specific values of the solute diffusion layer thickness at the dendrite tip frontier under different flow velocities are shown in Table 2. The solute diffusion layer thicknesses under convection could be quantitatively seen in the table.

Effect of melt forced flow on micro-segregation: In the usual production of castings, micro segregation refers to the composition difference between the center of the dendrite arm and the area among the dendrites. The size of the micro segregation could be expressed by segregation ratio S_R, which is the ratio of the lowest solute concentration at the dendrite arm and the largest inter dendritic solute concentration.

The segregation ratio values under different convection velocity are shown in Table 3. It can be seen in the table that segregation ratio of the dendrite increases with the increasing of the convection velocity. On the one hand, the solute was scoured from upstream to downstream under convection. More solute was scoured with increasing of the convection velocity. From the solute distribution in Fig. 1, as the flow speed increases, the maximum inter dendritic solute concentration becomes higher and higher. On the other hand, since the concentration of downstream dendrite frontier also increases and the temperature of liquidus decreases, the

Table 2: Thickness of concentration boundary layer at different flow rate

Position	Upstream dendrite tip				Downstream dendrite tip			
Flow velocities (m sec^{-1})	0.0 (δ_1)	0.01 (δ_2)	0.02 (δ_3)	0.03 (δ_4)	0.0 (δ_5)	0.01 (δ_6)	0.02 (δ_7)	0.03 (δ_8)
Diffusion layer thickness (μm)	0.59	0.45	0.35	0.31	0.59	1.22	1.66	1.79

Table 3: Segregation ratio at different flow rate

Flow velocities (m sec^{-1})	0.0	0.01	0.02	0.03
Segregation ratio S_R	11.85	12.21	12.66	13.64

concentration in the solid phase of dendrite is reduced. From the concentration distribution at the center of the dendrite in Fig. 2, the center of the downstream dendrite arm has the minimum concentration, which decreases with the increasing of the convection velocity.

CONCLUSION

The morphology of the dendrite growth and the distribution of the solute field are significantly influenced by the melt convection. With increasing of the convection speed, the growth of the dendrite is more asymmetric. The upstream dendrite growth rate is greater than that of the downstream. The secondary dendrite at upstream was more developed and the dendrite in normal direction was bias more serious to the upstream. The Si concentration of at the center of dendrite principal axis in the upstream becomes higher and higher, while that in the downstream is getting lower and lower and the solute concentration in the paste area surrounded by the dendrite is getting higher and higher.

In the upstream, with increasing of the convection speed, the concentration gradient at dendrite tip frontier increases and the thickness of the solute diffusion layer decreases. On the contrary, the concentration gradient decreases in the downstream and the thickness of the solute diffusion layer increases.

Because of the convection effect, the maximum solute concentration of the dendrite increases, while the minimum solute concentration of the decreases. The micro segregation of the dendrite also becomes more serious caused by the convection effect. The simulation results are consistent with solidification theory.

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