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STUDY ON THE MULTIPLE DENDRITE GROWTH OF Al – Si BINARY ALLOY USING PHASE – FIELD METHOD (PFM)

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Phase – field method offers the prospect of carrying out realistic numerical calculation on dendrite growth in metallic systems. The dendritic growth process of Al – 0,02mole % Si binary alloy was simulated by the coupling method of phase field and solute field. The effects of anisotropic parameters on the growth morphology of dendrite were studied. The results show that with the increase of the anisotropy magnitude, the secondary dendrite arms are more developed, and the dendrite tip is obvious oriented. For the multiple dendrite growth, the dendrites present the morphology from the tip splitting to the dendrite tip oriented. The multi dendritic branching and remelting states of Al – Si alloy were obtained and the directional solidification remelting and solute segregation were obtained under different anisotropic index conditions. And numerical simulations were conducted to investigate the growth of single and multiple dendrites under coupled conditions of phase field, solute field, and flow field.

Keywords: Al – Si alloy, solidification, dendritic, segregation, PFM

INTRODUCTION

The advantages of Al – Mg cast alloy are small density, high strength and toughness, and excellent corrosion resistance. When magnesium content is less than 5 %, magnesium is solid dissolved in the β' phase, and the alloy is asingle phase alloy. The crystallization temperature range of Al – Mgcasting alloy is wide and how to control the crystallization of Al – Mg alloy and obtain ideal microstructures is an interesting topic. One of the most powerful techniques to emerge in recent years for modeling solidification microstructures is PFM. PFM has been extensively used to simulate the formation of solidification morphology becauseof its advantage of avoiding the explicit boundary tracking needed to solve the classical sharp interface model. During the microstructure evolution of the cast alloy, the transition behavior of the dispersed interfacial layer is influenced by the external field and the molten poolstructure, which makes the cast microstructureshow rich dendrite morphology [1,2]. Acta Materialia has published a number of researcharticles on the effect of liquid solid interfacelayer transformation and precipitation of second phase on microstructure in recent years [3-5],which indicates that the effect of dispelrsedinterface layer on phase transition process has been paid more and more attention by domestic and foreign scholars, especially since the globally competitive materials genome project wasofficially implemented. Understanding the microstructure evolution mechanism, changing the genome of materials, designing the microstructure of materials, and then obtaining high performance materials have been widely concerned. The advantages of aluminum alloy are light weight, high specific strength and environmental protection, and aluminum alloy is a typical engineering structural material, which is widely used in military, aerospace, automobile manufacturing, 3C and other fields. In this paper, PFM is adopted into the micro structure calculation forthe dendritic growth of multiple dendrites and directional solidification of Fe – C binary alloy.

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PHASE FIELD MODEL

Phase – field model used in the paper was KKS model [6-8] for dilute binary alloy, and the solute controlling equation was coupled into the model to carry out a isothermal simulation. In the model, the variable $\varphi(x,y,t)$ is an ordering parameter at the position (x,y) and the time t, φ=1 means the alloy is solid and φ=0 means the alloy is liquid. The solid – liquid interface is expressed by the steep layer of φ connecting the value 0 and 1, and the phase field model can be described by:

$$\frac{\partial \varphi}{\partial t} = M(\varepsilon^2 \nabla^2 \varphi - f_\varphi) \tag{1}$$

$$\frac{\partial c}{\partial t} = \nabla \cdot (\frac{D(\varphi)}{f_{cc}} \nabla f_c) \tag{2}$$

Where M and ε are phase field mobility and gradient energy coefficient, respectively. f is the free energy density of the system, and the subscripts under f indicate the partial derivatives. $D(\varphi)$ is the diffusivity of solute as a

Table 1 **Thermophysical data for dilute Al - 0,02mole % Si alloy[9]**

Property	$\sigma(j\cdot m^{-1})$	$T_m(k)$	$V_m(m^3/mole)$	k^e	$D_1(m^2\cdot s^{-1})$	$D_2(m^2\cdot s^{-1})$	m_e
Al0,02mole%Si	0,093	933	$10,6\times10^{-6}$	0,807	$3,0\times10^{-}$	$1,0\times10^{-}$	939

function of phase field. Considering the effect of anisotropic interfacial energy, an energy form adopted by Kobayashi was used:

$$\varepsilon = \varepsilon_0(1+v\cos k(\theta-\theta_0)) \tag{3}$$

Where ε_0 is a parameter about interface width, θ is a angle between the normal to the interface and the *x–axis*, $\theta = \arctan(\varphi_y / \varphi_x)$, $\theta_0 = 2\pi/\varphi$, which is the angle between the crystallographic axis and xaxis; φ is a random number between 0 – 2π, v is the magnitude of anisotropy.

PHASE FIELD PARAMETERS

The phase field parameters of f and W are related to the interface energy σ and the interface width 2λ. From the definition of interface energy and interface thickness, ε and W can be determined.

$$\varepsilon = \sqrt{\frac{6\lambda}{2,2}\sigma} \tag{4}$$

$$W = \frac{6,6\sigma}{\lambda} \tag{5}$$

Phase field mobility M is related to the in terface kinetic coefficient b. It can be obtainedfrom the fact that the thin thickness is small compared with the diffusive boundary layer:

$$M^{-1} = \frac{\varepsilon^2}{\sigma}\left(\frac{RT}{V_m}\frac{1-k^e}{m^e}\beta + \frac{\varepsilon}{\sqrt{2w}D_i}\xi(c_S^e, c_L^e)\right) \tag{6}$$

$$\xi(c_S^e, c_L^e) = \frac{RT}{V_m}(c_L^e - c_S^e)^2 \times$$

$$\times\int_0^1 \frac{h(\varphi)[1-h(\varphi)]}{[1-h(\varphi)]c_L^e(1-c_L^e)+h(\varphi)c_S^e(1-c_S^e)}\cdot\frac{d\varphi}{\varphi(1-\varphi)} \tag{7}$$

Where m^e is the equilibrium slope of the liquids; k^e is the equilibrium partition coefficient and D_i is the diffusion coefficient in the interface region.

The two – dimensional simulations were performed at 903 K on an Al – 0,02mole % Si alloy system with thermos – physical data given in Table 1.

COMPUTATIONAL METHOD AND CONDITIONS

In the dendrite growth calculation, Isothermal computations were performed using thedilute solution model described above. In the calculation, governing equations were discret ized on uniform grids by using an explicit fin ite difference scheme. The two dimensional square calculation areas of 700 × 700 grids for phase field and solute field were meshed. The grid sizes of

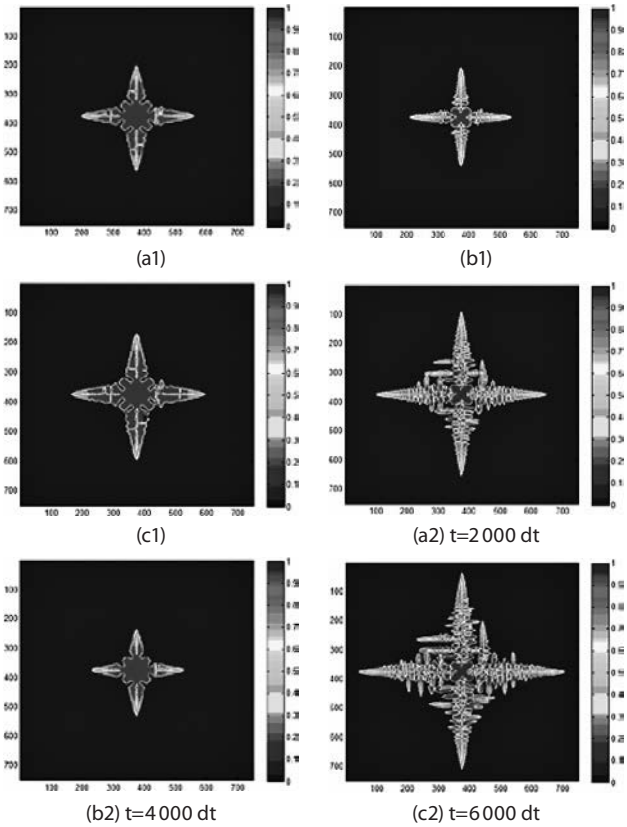

Figure 1 The dendrites growth effected by anisotropy: (a1-c1) the anisotropy magnitude is 0,04; (a2-c2) the anisotropy magnitude is 0,06

phase field and concentration field are $1,0 \times 10^{-8}$ m, ($dx = dy$, $dt = dx^2/5D_L$, the magnitude of anisotropy $v = 0,01$; magnitude of noise $w = 0,01$. In the multiple dendrites growth, five random small circle solid of 10 × 10 grids are initially put in the simulationarea as nucleation. To the directional solidification, the frozen temperature approximation [9-11] can be employed, and Neumann boundary condition was used to the simulation. The undercooling value was set 20 K in the two numerical simulations. The single dendrite growth is showed in Figure 1.

RESULTS AND DISCUSSION

In the corresponding figure of the microstructure evolution, the solidification front advances very slowly at the beginning from a droplet, and accelerates while the solidification is developing a cellular pattern, then the shape ofdendrites came out at last. As shown in Figure 1, the comparison of different dendrite patterns were carried out in the numerical simulateon, with the increasing of the anisotropy, we can see that the second dendrite arms became more developed, and the crystal structure is more developed in the large magnitude of anisotropy.

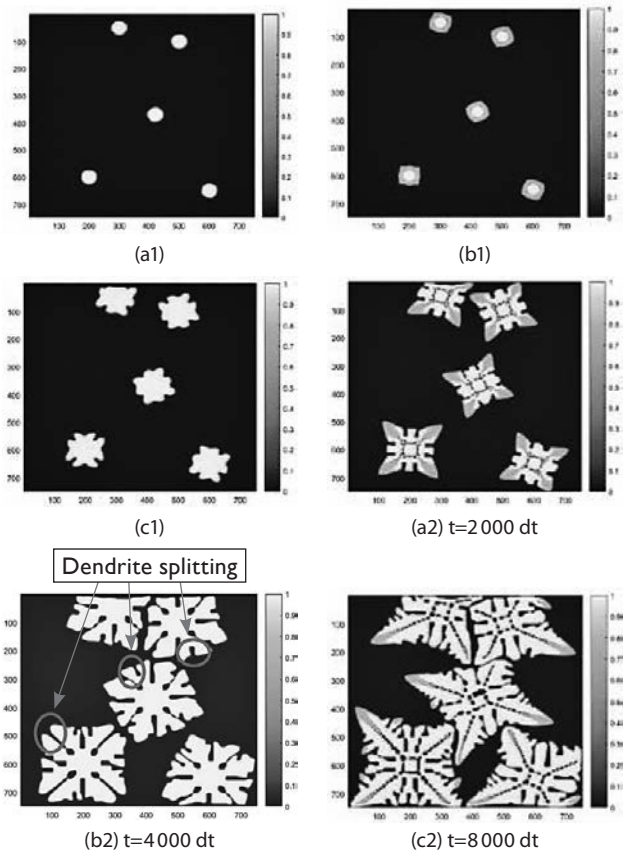

Figure 2 The multiple dendrites growth effected by anisotropy: (a1-c1) the anisotropy magnitude is 0,02; (a2-c2) the anisotropy magnitude is 0,04

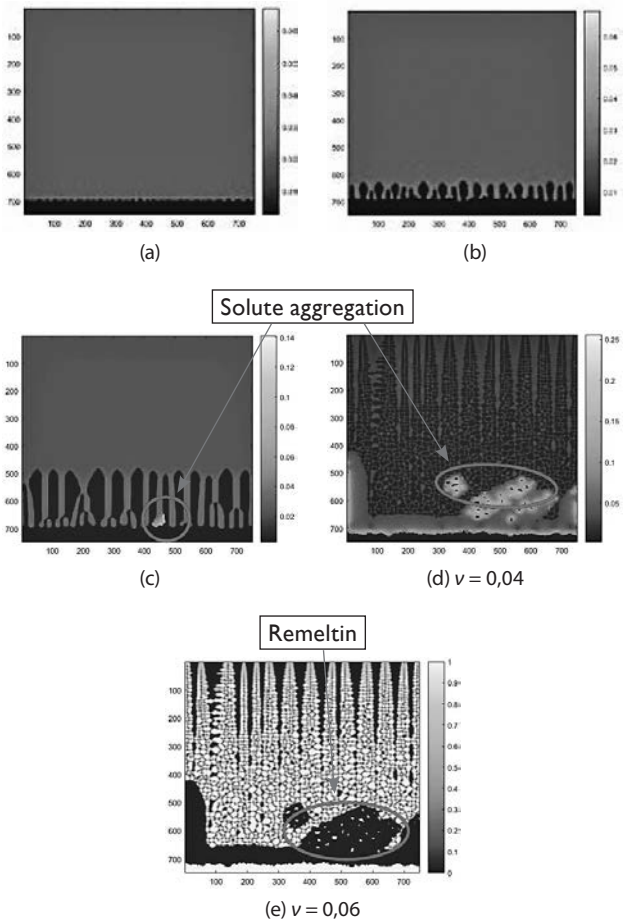

Figure 3 The solute field distribution in different magnitude of anisotropy: (a) theanisotropy magnitude is 0,04; (b) the anisotropy magnitude is 0,06

For the multiple dendrites growth, at the early stage, as shown in Figure 2 (a), (b), and (c),the crystallites with different orientation grew independently. With the increase of time, the grains begin to coalesce and impinge the adjacent grains. When the dendrites start to impinge, the dendrite growth is obviously inhibited. The competitive growth of these grains during solidification was observed. The simulated results showed that the solidification features are consistent with those observed based on the dendrite growth in transparent materials and also consistent with those observed based on metallographic examination of cast microstructures.

For the dendrite growth of direcional solidification, the solute field distribution is shown in Figure 3, the low concentration of Mg showed near the center line of the dendrites, because of the undercooling in the interface region,which is the driving force to the dendritic-growth, and the rate of diffusion of the solute solid phase lagged far behind the dendrite growthvelocity. For the solute redistribution, Mg concentration in the solid phase is lower than theinitial concentration of the melt, and the velocity of the liquid phase diffusion of the solute isless than the growth rate of the dendrite, the solidification of precipitated solute can not be sufficiently diffused into the liquid phase, therefore it enriched in branchescrystal forefront of the dendritic solidification interface region. The interface moving velocity is much higher than the diffusion velocity of the

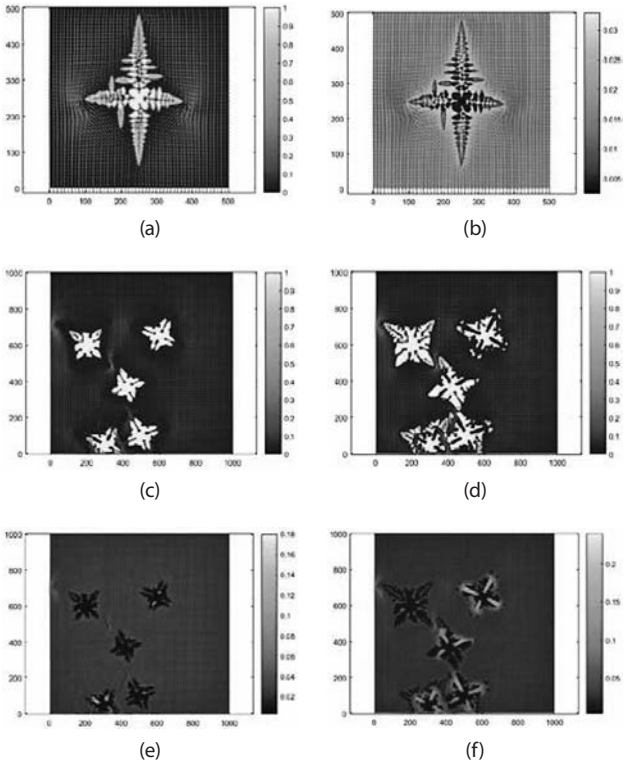

Figure 4 (a-b) Single dendrite growth phase field and solute field; (c-f) Phase and solute fields of multi dendritic growth

solute, so theconcentration gradient reach the maximum value in the dendrite tip zone. In terms of the interfacial region surrounded by crystal arm, the solute is not easy to diffuse to theliquid phase, the solute concentrated in the area, and the necks of dendrites were shrinked in the zone below. With the increasing of the anisotropy, dendrite tip radius became smaller, and thecrystal structure is more uniform and dense.

The effect of flow field action on solute diffusion during solidification was considered,and the microscopic flow field was coupled to the solute field equation by modifying the solute gradient term near the solid – liquid interface. Therefore, the solute field equation under forced convection becomes.

$$\frac{\partial c}{\partial t} = \nabla \cdot \left(\frac{D(\varphi)}{f_{cc}} \nabla f_c \right) + \vec{u} \nabla c \qquad (8)$$

where $D(\varphi)$ is the solute diffusion coefficient, $D(\varphi) = = D_L + h(\varphi)(D_S - D_L)$, D_S and D_L are the solute diffusion coefficients of the solid and liquid phases, respectively, f is the free energy density of the metal system, and the subscript c represents the partial derivative of f, $\vec{u}$ is a parameter related to the flow velocity.

CONCLUSIONS

The multiple dendrites growth showed theimpingement of arbitrarily oriented grains, andthe grains began to impinge and coalesce the adjacent grains with time going on, which madethe dendrite growth inhibited obviously. In the directional solidification process, found that the neck of columnar dendrite root remelted in low magnitude of anisotropy. With the increasing of the anisotropy, the dendrit tip radiusbecame smaller, the orientation was strengthened, and the crystal structure is more uniform and dense.

The multi dendritic branching and meltingstates of Al – Si alloy were obtained under different anisotropic index conditions, As the anisotropy index increases, the phenomenon of branching at the top of multiple dendrites disappears. The directional solidification remelting and solute segregation of Al – Si alloy were obtained under different anisotropic index conditions, As the anisotropy index increases, the bottom of the directionally solidified columnar dendrites begins to remelt, and the solute drag effect is obvious. The numerical simulat ions were conducted to investigate the growth of single and multiple dendrites in Al – Si alloy under coupled conditions of phase field, solute field, and flow field. Under the influence of the coupled flow field, the growth of columnar dendrites in the countercurrent direction is significantly better than that in the downstream direction.

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