Materials Science Forum *Online: 2007-10-02*
ISSN: 1662-9752, Vols. 561-565, pp 1787-1792
doi:10.4028/www.scientific.net/MSF.561-565.1787

Numerical Modeling of Microstructure Evolution and Dendrite Growth for Al-Si Alloy Casting during Low Pressure Die Casting

B. Li[1,a], Q. Y. Xu[1,b], B. C. Liu[1,c]

[1]Key Laboratory for Advanced Materials Processing Technology (MOE), Department of Mechanical Engineering, Tsinghua University, Beijing 100084, China

[a]libin03@mails.tsinghua.edu.cn, [b]scjxqy@tsinghua.edu.cn, [c]liubc@tsinghua.edu.cn

Keywords: Microstructure simulation, Aluminum alloy, Low pressure die casting

Abstract. A modified Cellular Automaton model was presented to simulate the evolution of dendritic microstructure in low pressure die casting of Al-Si Alloy, which accounted for the heterogeneous nucleation, the solute redistribution both in liquid and solid, the interface curvature and the growth anisotropy during solidification. The free growth of single equiaxed dendrite and the evolution of multi dendrites with various crystallographic orientations were predicted. The variation of the dendrite tip velocity and local solute concentration at the solid/liquid interface were analyzed. The grain morphology of aircraft turbine wheel casting at different specimen points were predicted and compared with experimental results.

Introduction

Solidification microstructure can affect the performances of the final castings to a great extent. So it is very important to better understand and control the formation of solidification microstructure. Besides physical experiments and analytical techniques, numerical simulation is a very powerful tool to study microstructure evolution because of its high efficiency and low cost.

In recent decades, microstructure simulation of aluminum alloys during solidification has been studied extensively by many groups in the world from meso-scale to micro-scale. Celluar Automaton models[1-7] and Phase Field models[8,9] are two kinds of ones which are applied most popularly till now. Phase field (PF) models can simulate the kinetics of dendrite growth and realistic dendritic morphology using entropy or free energy formulation. However, PF models demands a large number of computer resources, so it can only simulate a few dendrites in a smaller domain. CA models are closer to practical application because it is simpler to program and solve in a PC and the simulated domain is larger.

In this paper, the solidification of Al-7wt%Si-0.5wt%Mg alloy during low pressure die casting was analyzed, and nucleation model of the alloy was established based on a number of experimental data. A modified CA method coupled with finite difference method was used to simulate the evolution of the alloy microstructure. The preferential growth orientation, the solute redistribution in both liquid and solid, the solid/liquid interface curvature and the growth anisotropy were all taken into account in the model, reproducing the growth of multi dendritic grains with different crystallographic orientation. The grain size at different position of the aircraft turbine wheel casting were predicted and compared with experimental results.

Model description

Alloy Solidification Process Analysis. The equilibrium structure of Al-7wt%Si-0.5wt%Mg is primary α Al, Al-Si eutectic and Mg_2Si reinforced phase. The content of Mg_2Si is usually less and it is distributed dispersedly so that it is hard to identify [10]. On the other hand, based on the calculated results of THERMO-CALC software, at the end of binary eutectic transformation L→Al+Si, solid fraction of primary and eutectic microstructure is already above 95 percent. Then ternary eutectic

transformation begins and complex phases can appear. So the solidification process of Al-7wt%Si-0.5wt%Mg alloy can be simplified into that of Al-7wt%Si alloy, which can still represent the main characteristic of microstructure evolution. The pressure under which the alloy solidifies is below 0.1MPa for low pressure die casting, so the influence of the pressure on solidification process and final microstructure can be neglected.

Nucleation Model. The continuous nucleation model based on Gaussian distribution was used popularly for Aluminum alloy solidification[11,12]. Grain density $n(\Delta T)$ at one certain undercooling is calculated as follows:

$$n(\Delta T)=\int_0^{\Delta T}[1-f_s(\Delta T)]\frac{dn}{d(\Delta T)}d(\Delta T) \tag{1}$$

$$\frac{dn}{d(\Delta T)}=\frac{n_{\max}}{\sqrt{2\pi}\Delta T_\sigma}\exp[-\frac{1}{2}(\frac{\Delta T-\Delta T_N}{\Delta T_\sigma})^2] \tag{2}$$

Where ΔT is the actual undercooling, $n_{\max}$ is the maximum density of nucleation sites, ΔT_N is the mean nucleation undercooling, ΔT_σ is the standard deviation of the distribution.

However, for the solidification process under practical processing condition, it is not exact to reflect the characteristic of nucleation process if following the previous model parameters completely. So it is necessary to carry through numerical statement and analysis based on a number of experimental data, and then the related experimental nucleation parameters can be concluded. Twelve sets of experiments for plate- shaped and step-shaped castings were designed in the present study, and cooling rate and grain size at every specimen position were measured. The final calculated results based on statistics and analyses for acquired experiment data are as follows: $n_{\max}=7.0\times10^9$; $\Delta T_N=20$ K; $\Delta T_\sigma=0.1$ K.

Dendrite Growth Model. After the primary α Al begins to nucleate, it grows with dendritic shape for alloy equiaxed solidification condition. As the dendrite grows, latent heat and solute are released into the solid/liquid interface. Besides, the dendrite shape also changes the interface curvature. The changing thermal/solute field and interface curvature all influence the equilibrium interface undercooling/movement. So the heat and mass transport will continue through the whole solidification process. Solid/liquid interface equilibrium composition during alloy solidification process was calculated in this paper based on thermal and solutal conservation. Constitutional undercooling, curvature undercooling and anisotropy factor at solid/liquid interface were considered to establish interface kinetics model. Microstructure evolution was simulated through solving governing variables such as temperature, concentration, solid fraction and interface velocity. Modified CA method can describe not only grain profile, but also dendrite morphology with different crystallographic orientations. The related governing equations are as follows.

(1) Equilibrium composition and solute conservation at solid/liquid interface

The local interface equilibrium composition and solute conservation are calculated by the following equations:

$$C_L^*=C_0+\left(T^*-T_L+\Gamma\bar{k}f(\varphi,\theta)\right)/m_L \tag{3}$$

$$C_S^*=k_0C_L^* \tag{4}$$

$$v_n^*C_L^*(1-k)=D_L\left(\frac{\partial C_L}{\partial x}+\frac{\partial C_L}{\partial y}\right)-D_S\left(\frac{\partial C_S}{\partial x}+\frac{\partial C_S}{\partial y}\right) \tag{5}$$

Where C_S^* is the solid equilibrium composition at the solid/liquid interface, k_0 is the equilibrium partition ratio, v_n^* is the normal velocity of the solid/liquid interface.

(2) Interface curvature and anisotropy factor at solid/liquid interface

The variation of the interface curvature can directly reflect dendrite morphology. Besides, it can result in the change of the temperature at solid/liquid interface (curvature undercooling), which affects the growth of dendrite front. For the CA cell at the solid/liquid interface, its curvature is determined by the solid fraction of itself and its neighborhood cells. The growing dendrites in the simulated domain have different preferential growth direction (crystallographic orientation) which is determined by crystal anisotropy including the influence of interface energy and growth kinetics[2,5,13]. The interface curvature and anisotropy factor are calculated by the following equations.

$$\bar{k} = \frac{1}{l}\left(1 - 2\frac{f_S + \sum_{k=1}^{N} f_S(k)}{N+1}\right) \tag{6}$$

$$f(\varphi,\theta) = 1 + \gamma\cos[4(\varphi - \theta)] \tag{7}$$

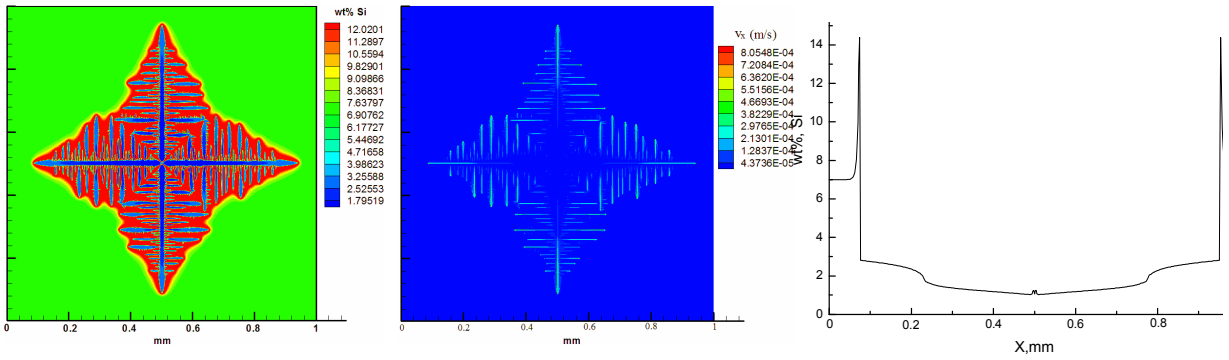
$$\varphi = \arccos\left(\frac{\partial f_s / \partial x}{\left[(\partial f_s / \partial x)^2 + (\partial f_s / \partial y)^2\right]^{1/2}}\right) \tag{8}$$

Where N is the number of neighbors of the interface cell. 24 cells can be counted if two-layer cells around the interface cell are considered in 2D, which means N=24. γ is the anisotropy factor and here equals to 0.04, $f(\varphi,\theta)$ is a function describing the anisotropy of the surface tension, φ is the angle of the normal to the interface with respect to the reference axis, θ is the angel of the preferential growth direction (crystallographic orientation) with respect to the reference axis.

In this paper, the grids rotating and coordinate transformation method was used to overcome the anisotropy introduced by the mesh of square cells. The details are described in the reference[7].

Results and discussions

Single dendrite growth. The simulation of single dendrite growth for Al-7wt%Si alloy were performed in a domain consisting of 500×500 square meshes with mesh length of 2 μm. One crystal nucleus was set at the center of the domain and grew at a constant cooling rate 70 k/s. Fig. 1 shows the simulated dendrite morphology when the growth time was about 2.96 s. Fig.1 (a), (b), (c) is solute concentration field, dendrite tip growth velocity field and Si concentration distribution along the horizontal center line of the domain, respectively. As shown in Fig.1, the solute concentration decreases with bigger gradient in liquid, while smaller in solid. The solute accumulates most at the solid/liquid interface because large amounts of solute are released into the adjacent liquid when interface cells solidify and the solute diffuses slowly in liquid. The concentration in liquid decreases quickly. The diffusion is slower in solid, so the concentration changes slowly in solid. Due to solute pileup between the dendrites, the velocity at the tip of dendrites is higher than that between the dendrites.



(a) solute concentration field (b) dendrite tip velocity field (c) Si concentration at the center line

Fig. 1 Simulated dendrite morphology of Al-7wt%Si alloy

Fig. 2 shows the variation of dendrite tip growth and solute concentration in liquid and solid with time. As shown in Fig.2, at the beginning of the solidification, the tip velocity is close to zero because the undercooling is very small. As the solidification proceeds, the undercooling increases gradually and the tip velocity increases correspondingly. At the same time, dendrite tip liquid composition also increases. When the growth time was around 2.96 s, the growing dendrite tip is close to the boundary of the simulated domain and the tip velocity becomes the biggest, and after this, decreases rapidly due to too much solute pileup as well as boundary obstruction.

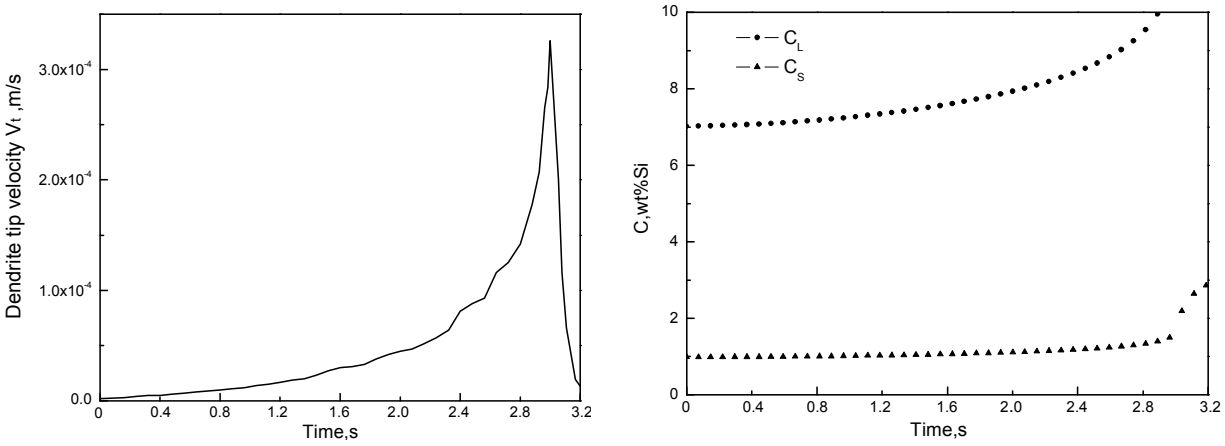
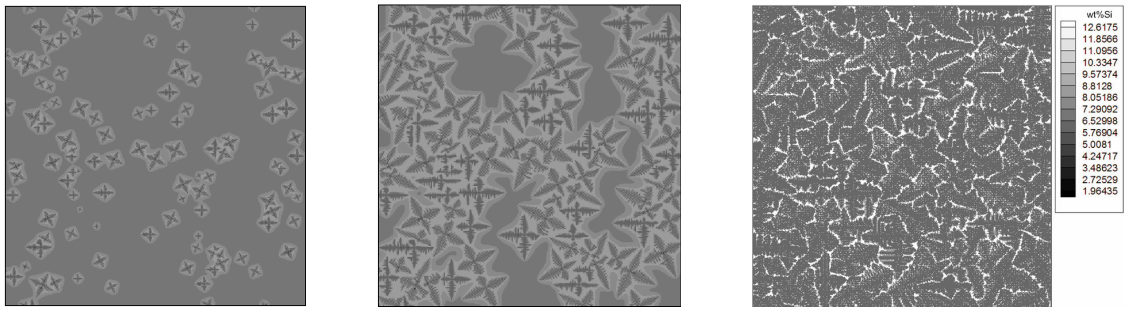


Fig. 2 Variation of dendrite tip velocity (left) and dendrite tip liquid and solid composition (right) with time

Multi-dendrites growth. The simulation were performed in a domain consisting of 500×500 square meshes with mesh length 2 μm. The temperature in the entire domain was assumed to be homogeneous and cooled down with a constant rate 70 k/s. Fig.3 shows the growth evolution of multi-dendrites with different crystallographic orientations. As shown in Fig.3, at the initial stage of solidification, equiaxed crystal nuclei begin to appear randomly in the undercooled liquid with different crystallographic orientations, and then grow with dendritic shape. Secondary dendrite arms grow on the primary dendritic arms and even ternary arms appear. As the solidification proceeds, the solutes are rejected from the solid/liquid interface into the remaining liquid gradually. The solute concentration between the dendrites is higher and higher. When the concentration is up to 12.6%, the dendrites stop growing. The eutectic structures finally form at grains boundaries and the interdendrite regions.



(a) t=0.03 s (b) t=0.09 s (c) t=0.63 s

Fig.3 Multi-dendrites growth of Al-7wt%Si alloy

Microstructure simulation application in aircraft turbine wheel. To validate the model presented in this paper, an aircraft turbine wheel casting made of Al-7wt%Si-0.5wt%Mg alloy was selected to compare simulation results of solidification microstructure with those in experiment. The pouring temperature is 710°C; the supercharged pressure is 0.05MPa. The size of the casting is 30 mm (height)×135 mm (diameter) and the thickness of the thinnest position is only 2 mm. The number of the casting cells and the chill cells is 157,558 and 133,560, respectively and the total number of macro cells including sand mould cells is 2,073,600. Seven 5 mm×5 mm specimens were taken from the

longitudinal section at the center of the wheel and indexed as P1-P7 in order. The casting shape and the positions of the specimens are schematically shown in Fig.4.

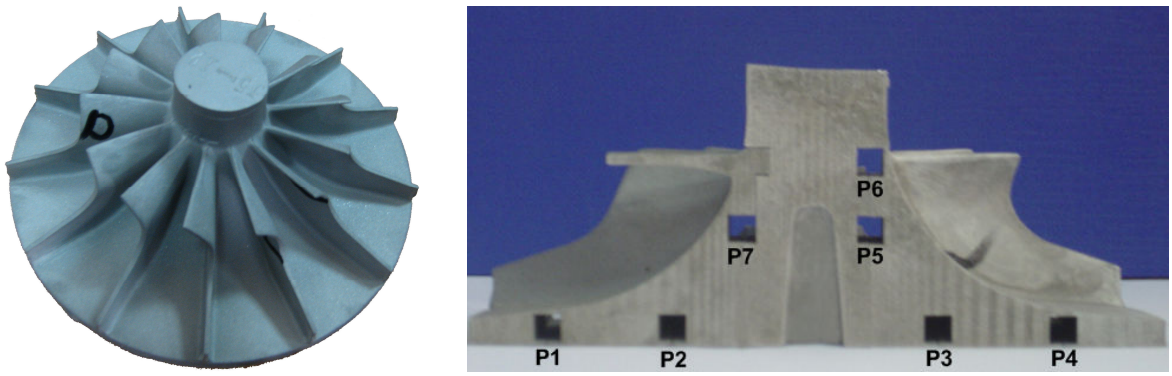


Fig.4 Schematics of aircraft turbine wheel casting (left) and specimen positions (right)

Modified CA model coupled with finite difference method was used to simulate the evolution of the microstructure of the above casting. The macro cell size for heat transfer calculation is 1 mm×1 mm×1 mm and the 2D micro cell size for microstructure calculation is 2 μm×2 μm. Fig.5 is the comparison between the simulated and experimental microstructure at different specimen point of the aircraft turbine wheel casting. The order of cooling rate of specimen positions from fast to slow is: P1>P3>P6>P5. As shown in Fig.5, grain size is smaller and secondary dendrite arm space is also smaller as the cooling rate increases. These can be understood due to the fact that the increase of the cooling rate will lead to the increase of the undercooling and the number of nuclei in one certain domain, which causes the grains refining.

Conclusions

(1) The dendrite growth model was established considering the solute redistribution in both liquid and solid, the solid/liquid interface curvature, the growth anisotropy, reproducing the growth of multi dendrites with different crystallographic orientation. The variation of the dendrite tip velocity and local solute concentration at the solid/liquid interface were analyzed.

(2) A modified CA method coupled with finite difference method was presented to simulate the evolution of Al-7wt%Si alloy microstructure. The grain morphology at different position of the aircraft turbine wheel casting were predicted and compared with experimental results and they agreed with each other well.

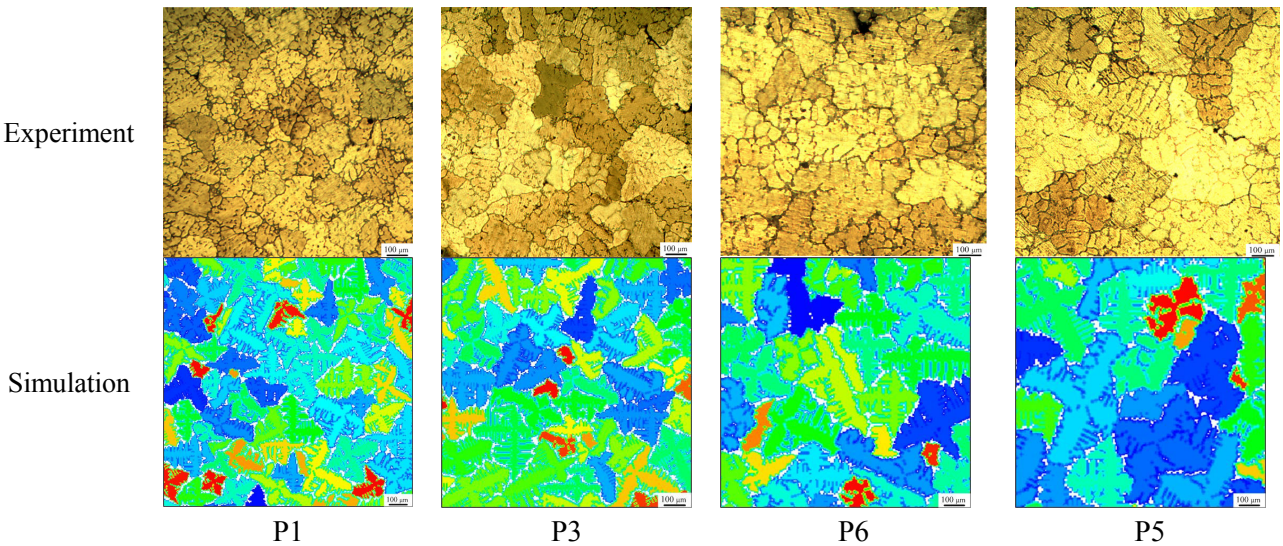


Fig.5 Comparison of simulated and experimental microstructure for turbine wheel casting

References

[1] Gandin Ch-A, Rappaz M. Acta Mater. Vol. 45, (1997), p. 2187

[2] L. Nastac, Acta Mater. Vol. 47, (1999), p. 4253

[3] M. F. Zhu, and C. P. Hong. ISIJ Int. Vol. 41, (2001), p. 992

[4] M. F. Zhu, and C. P. Hong. ISIJ Int. Vol. 42, (2002), p. 520

[5] L. Beltran-Sanchez, and D. M. Stefanescu. Metall Mater Trans A. Vol. 34, (2003), p. 367

[6] H. B. Dong, and P. D. Lee. Acta Mater. Vol. 53, (2005), p. 659

[7] Y. Liu, Q. Y. Xu, and B. C. Liu. Tsinghua Science and Technology. Vol. 11, (2006), p. 495

[8] C. Beckermann, Q. Li, X. Tong. Science and Technology of Advanced Materials. Vol. 2, (2001), p. 117

[9] I. Steinbach, C. Beckermann, B. Kauerauf, Q. Li, J. Guo. Acta Mater. Vol. 47, (1999), p. 971

[10] B Closset, J E Gruzleski. AFS Transaction. Vol. 90, (1982), p. 453

[11] P. Thévoz, J. L. Desbiolles, and M. Rappaz. Metall Mater Trans A. Vol. 20, (1989), p. 311

[12] C. A. Gandin, C. Charbon, and M. Rappaz. ISIJ Int. Vol. 35, (1995), p. 651

[13] L. Beltran-Sanchez, and D. M. Stefanescu. Metall Mater Trans A. Vol. 35, (2004), p. 2471