Effect of thermal convection on columnar-to-equiaxed transition during solidification of Al-Cu alloy

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Abstract: To investigate the effect of three-dimension (3D) thermal convection on columnar-to-equiaxed transition (CET), the CET transition during the solidification of an Al-Cu alloy was simulated by 3D cellular automaton model coupled with the finite element method (CAFE). The thermal convection in the liquid phase was considered. The results show that the thermal convection in the liquid phase promotes the CET. When the convection is present, the temperature gradient at the start position of CET increases and the growth velocity of columnar dendrite decreases. The convection influences the formation of elongated equiaxed grain through changing the local temperature gradient and dendritic growth velocity.

Key words: columnar-to-equiaxed transition; Al-Cu alloy; simulation; convection

CLC numbers: TG146.21

Document code: A

Article ID: 1672-6421(2018)05-358-05

Columnar-to-equiaxed transition (CET) is a normal phenomenon during the solidification of alloys^[1]. A great deal of effort has been devoted for many years to understand the mechanism of the CET because the dendrite structure can effect the properties of casting. In 1984, Hunt developed the first CET model^[2]. Since then, many numeric models have been developed to predict the CET during the solidification of alloys^[3-15]. Hunt's model assumed that the equiaxed grains can nucleate and grow in the undercooled region in front of columnar dendrites. If the volume fraction occupied by equiaxed grains is large enough when the columnar front arrives, they will block the progress of the columnar front. Hunt's model is used extensively in solidification models. However, it does not predict a gradual transition from elongated equiaxed grains to truly equiaxed ones. Gäumann et al.^[3] developed a theoretical model based on Hunt's model to predict the CET transition in many processes. The model takes into account the

local concentration and the local undercooling at low and high interface velocities. Therefore, the model is appropriate for predicting the CET transition in the rapid solidification. The development of numerical simulation provides a powerful method for predicting the CET in the solidification of alloys. Zhu and Smith^[4,5] developed an improved Monte Carlo model reported by Brown and Spittle^[6] because the previous model was difficult to use in the study of the solidification of an alloy system. The model was applied to predict the multi-directional freezing of a two-dimensional (2D) ingot of Al-4.5wt%Cu. The cellular automaton model provides a simple means for calculating the grain structure. Gandin and Rappaz^[7] first predicted the dendritic grain structures in solidification processes by a fully coupled finite element-cellular automaton model (CAFE). Dong and Lee^[8,9] developed a cellular automaton model coupled with finite difference method (CAFD) to simulate the CET during the solidification of an Al-3wt.%Cu alloy. The simulated results were in agreement with experimental observations. In order to take into account the different scale lengths existing in a dendritic structure, Wang and Beckermann^[10] simulated the CET transition by a multiphase approach. The calculated CET positions are in a good agreement with measurements in a (1D) ingot cast under well-controlled conditions. Badillo and Beckermann^[11] simulated the CET transition in directional solidification of alloys by

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Received: 2018-03-20; Accepted: 2018-04-08

the phase-field method. The results qualitatively agree with a previously developed analytical model of the CET. However, none of these studies considered the effect of convection.

Convection has an obvious effect on dendritic structure formation^[12]. So, it is necessary to couple the dendritic growth kinetic calculation with the fluid flow in the liquid phase. Many researchers have focused on the microstructure formation under the convection^[12-16]. The effects of heat transport, convection and solute mass on grain structure were studied by Reinhart^[12]. The position of CET in the samples as well as elongation of the grains is well predicted by using 2D CAFE model. Willers et al.^[14] carried out an experiment to reveal the influence of a rotating magnetic field (RMF) on the unidirectional solidification of Pb-Sn alloys. They found that the convection in the melt generated by the RMF reduced the temperature gradient ahead of the solidification front and promoted the CET transition. Spinelli et al.^[15] studied the influence of melt convection on the CET transition by the theoretical and experimental approach. They founded that the melt convection favors the CET transition in conditions of downward solidification. Banaszek et al.^[16] simulated the CET and liquid flow in directional solidification controlled by the diffusion. Results show that natural thermal convection can promote equiaxed solidification. However, to date, the simulation was carried out in a 2D sample. The three-dimension (3D) convection occurs during the solidification of the actual castings. How the 3D convection affects the CET transition has not been reported.

In order to better understand the effect of 3D convection on the CET transition, the CET transition during solidification of an Al-3wt.%Cu alloy was investigated by the cellular automaton coupling with the finite element method because it had a much higher computational efficiency compared with other models. The microstructural formation of Al-3wt.%Cu alloy ingots with different diameters was simulated. The three-dimension convection caused by non-uniform temperature in liquid was considered.

1 Numerical method

The CAFE module of the software Pro/Cast was used to simulate the dendrite growth. The convection caused by the un-uniform temperature in the liquid phase was calculated. The floating grains coming from the upper surface of the casting and crystal multiplication due to thermo-mechanical fragmentation promoted by the convection are neglected because the magnitude of convection is very small.

The post-processing mode was used to calculate the dendrite growth. The calculation process was: (1) calculating the temperature field and the fluid flow field; (2) calculating nucleation and dendrite growth by CAFE model.

1.1 Calculation of fluid flow and heat transport

Navier-Stokes equations are used to calculate fluid flow in the liquid phase. The equation of continuity is:

$$\nabla \cdot (\rho u) = 0 \quad (1)$$

Navier-Stokes equation is:

$$\frac{\partial(\rho u)}{\partial t} + \nabla \cdot (\rho u u) = -\nabla p + \nabla \cdot (\mu \nabla u) + (\rho - \rho_0)g \quad (2)$$

where u is the velocity vector ($\text{m}\cdot\text{s}^{-1}$), t is time (s), ρ is the density ($\text{kg}\cdot\text{m}^{-3}$), μ is the viscosity (P), p is the hydrostatic pressure (Pa), ρ_0 is the density at the reference temperature and pressure ($\text{kg}\cdot\text{m}^{-3}$), g is gravity acceleration ($\text{m}\cdot\text{s}^{-2}$).

The governing equation for heat distribution by the convection and the diffusion is given by:

$$\frac{\partial T}{\partial t} + \nabla \cdot (uT) = -\nabla \cdot (\alpha_1 \nabla T) + Q \quad (3)$$

where T is temperature (K), α_1 is the thermal diffusion coefficient ($\text{m}^2\cdot\text{s}^{-1}$); Q is the source term accounting for the release of the latent heat.

1.2 Nucleation rate

The density of the equiaxed dendrite ahead of the solid/liquid (S/L) interface was calculated by the continuous distribution model. The density of nucleus is given as^[17]:

$$\frac{dn}{d(\Delta T)} = \frac{n_{\max}}{\sqrt{2\pi} \cdot \Delta T_\sigma} \exp\left[-\frac{1}{2} \left(\frac{\Delta T - \Delta T_0}{\Delta T_\sigma}\right)^2\right] \quad (4)$$

where, n is the density of nucleus (m^{-3}), ΔT is the total undercooling (K), $n_{\max}$ is the total density of available particles (m^{-3}), ΔT_0 is the mean value of the distribution (K), and ΔT_σ is the standard deviation (K).

1.3 Growth of dendrite

The S/L interface velocity (v) was calculated by using the KGT model^[18]:

$$v = \alpha \Delta T^2 + \beta \Delta T^3 \quad (5)$$

where, α and β are coefficients ($\text{m}\cdot\text{s}^{-1}\cdot\text{K}^{-2}$).

2 Results and discussion

The microstructural evolution during the solidification of Al-3wt.%Cu alloy was simulated. The parameters used in the present study are listed in Table 1. The size of samples are 10, 15, 20 and 25 mm in diameter, respectively, and 50 mm in height. The heat transfer coefficient of the bottom surface of the

Table 1: Parameters of Al-Cu alloy

Symbol	Unit	Value
α	$\text{m}\cdot\text{s}^{-1}\cdot\text{K}^{-2}$	1.16633
β	$\text{m}\cdot\text{s}^{-1}\cdot\text{K}^{-3}$	4.604×10^{-7}
$n_{\max}$	m^{-3}	1.0×10^9
ΔT_0	K	0.75
ΔT_σ	K	0.1
μ	P	0.014
α_1	$\text{m}^2\cdot\text{s}^{-1}$	6.37×10^{-5}
ρ_0	$\text{kg}\cdot\text{m}^{-3}$	2,780

sample is $7.5 \times 10^2 \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$. The other surfaces are insulated. At the initial stage, the melt is stationary and the initial temperature is uniform. The initial temperature of the alloy is 1,025 K. In the solidification process, the temperature of the melt becomes non-uniform, which results in the inhomogeneity of melt density. As a consequence, the thermal convection is generated by the density differences in the fluid. The thermal convection influences the temperature field. This changes the local temperature gradients, thus altering the dendritic growth.

2.1 Flow pattern

The calculated flow patterns in the bulk liquid ahead of the S/L interface are shown in Fig. 1. The upper row of Fig. 1 shows flow patterns in longitudinal sections, and the lower row of Fig. 1 shows flow patterns in cross sections (sliced along the dashed line shown in the upper row of Fig. 1). It can be seen that with the increase of the sample diameter, the flow intensity increases. For a given alloy system, the flow intensity can be characterized by the Rayleigh number. The Rayleigh number Ra_T in upward solidification system is given as [19]:

$$Ra_T = \frac{g\beta_T G_H d^4}{\nu \alpha_1} \quad (6)$$

where, ν is the kinematic viscosity ($\text{m}^2 \cdot \text{s}^{-1}$); β_T is the temperature expansion coefficient (K^{-1}); G_H is radial temperature gradient ($\text{K} \cdot \text{m}^{-1}$) and d is the diameter of sample (m). Equation (6) indicates that the flow intensity is in proportion to four squares of the diameter of sample. It means that the effect of the sample diameter on the flow intensity is more significant than that of other factors. Therefore, the flow intensity increases with the increase of the sample diameter.

Figure 1 shows that in three dimensions, the flow is not only along the axial direction, but also along the radial direction. It is difficult to analyze the effect of flow on dendrite growth and CET under the such complex situation. Therefore, numerical calculation of the flow in 3D is very necessary to investigate the effect of flow on dendritic growth.

Fig. 1: Flow vector in liquid: (a) $d = 10 \text{ mm}$; (b) $d = 15 \text{ mm}$; (c) $d = 20 \text{ mm}$; (d) $d = 25 \text{ mm}$

2.2 Dendritic structures

The temperature gradient and dendritic growth velocity at

the position of the start and the end of CET are calculated and drawn in Fig. 2. In Fig. 2 the transition line between the columnar dendrite and the equiaxed dendrite obtained using the Hunt model [2] (solid line) and numerical results [3] (dashed line) are included. The top left corner shows the equiaxed dendrite zone. The lower right corner shows the columnar dendrite zone. It can be seen from Fig. 2 that when the convection is absent, the equiaxed dendrites are obtained in the columnar dendrite zone predicted by using Hunt model. When the convection is present, the calculated results are in a good agreement with the Hunt model and the numerical results from Ref. [3]. And, when convection is present, the temperature gradient at the start of CET increases and the columnar dendrite growth velocity decreases. This is because the convection influences on the thermal field through the advection of heat. The fluid flows from the high temperature zone to the S/L interface as shown in Fig. 1. Therefore, the undercooling ahead of the S/L interface decreases. This leads to the columnar dendrite growth velocity decreases. On the other hand, the temperature in the liquid phase tends to be uniform when the convection occurs, the formation of the equiaxed grains in liquid becomes easier accordingly.

Fig. 2: Comparison of simulated results with the Hunt model [2] and numerical results [3]

Calculated dendritic structures are shown in Figs. 3 and 4. It can be seen that the columnar dendrite transitions to the equiaxed in the solidification. Figures 3 and 4 also show that the transition between columnar and equiaxed grains is gradually from the columnar to the elongated “equiaxed” grains (shown in the rectangle zone in figures), to truly equiaxed grains. When convection is absent, there is an elongated equiaxed grain zone, as shown in Fig. 3(a) and (b), and there is no elongated equiaxed grain zone in Fig. 3(c) and (d). When the convection is considered, there is no elongated equiaxed grain zone in Fig. 4(a), (b) and (d), however, Figure 4(c) shows an elongated equiaxed grain zone. Dantzig and Rappaze [17] introduce a shape factor or elongation factor to analyze the formation of elongated equiaxed grain. The shape factor S is a function of the temperature gradient, velocity of the isotherms, for a particular set of thermal nucleation parameters and a specific growth kinetics law:

$$S = \frac{R_g^0(t_i)}{R_g^\pi(t_i - L/v_T)} > 1 \quad (7)$$

where, $R_g^0(t)$ and $R_g^\pi(t)$ are distances measured from the nucleated position of grain to the boundary of grain along the direction and the opposite direction of isothermal movement (m), respectively. $R_g^0(t)$ and $R_g^\pi(t)$ are the function of the undercooling and temperature gradient of the S/L interface. t_i is the impinge time of the neighbor grains (s). $L = n_g^{-1/3}$, and n_g is the density of nucleation sites (m^{-3}). v_T is the isotherm velocity ($\text{m} \cdot \text{s}^{-1}$).

When S is close to 1, the grains are truly equiaxed. The large value of S corresponds to columnar grains. In the present simulations, the temperature gradient and dendritic growth velocity are changed with the solidification process. If the local temperature gradient and isotherm velocity make the value of S large enough, the elongated grains will form, as shown in Fig. 3(a) and (b). When the convection is present, the temperature

field was modified by the convection. There was no elongated grain zone in samples with diameters of 10 mm and 15 mm, while there is an elongated grain zone in sample with a diameter of 20 mm, as shown in Fig. 4(c).

Figure 5 shows the start position of CET measured from the bottom of the sample. It can be seen that the start position of CET is lower when the convection is present. Therefore, even though the floating grains coming from the upper surface of the casting and crystal multiplication caused by thermo-mechanical fragmentation are not considered, the convection promotes the CET. The equiaxed structures are promoted due to the convection tendency to decrease the thermal gradient in the liquid^[17]. Figure 6 shows the calculated temperature field at solidification time of 15 s. The isothermal was no longer horizontal impacted by the convection. The temperature gradient ahead of the S/L interface at solidification time of 15 s is shown in Fig. 7. It can be seen that the temperature gradient ahead of

Fig. 3: Calculated dendrite structures when convection is absent: (a) $d = 10$ mm; (b) $d = 15$ mm; (c) $d = 20$ mm; (d) $d = 25$ mm

Fig. 4: Calculated dendrite structures when convection is present: (a) $d = 10$ mm; (b) $d = 15$ mm; (c) $d = 20$ mm; (d) $d = 25$ mm

Fig. 5: Calculated position of CET

Fig. 6: Calculated temperature field at solidification time of 15 s: (a1), (a2) $d = 10$ mm; (b1), (b2) $d = 15$ mm; (c1), (c2) $d = 20$ mm; (d1), (d2) $d = 25$ mm

the S/L interface decreases when the convection is present. This is because the convection can increase the transport of heat.

Fig. 7: Temperature gradient ahead of S/L interface at solidification time of 15 s

3. Conclusions

The CET transition during the solidification of an Al-Cu alloy was simulated by using a three-dimension (3D) cellular automaton model coupled with the finite element method (CAFE). The natural convection caused by the non-uniform temperature in liquid phase is considered. The results show that the convection in the liquid phase promotes the CET. When the convection is present, the temperature gradient at the start of CET increases and the growth velocity of columnar dendrite decreases. Convection influences the formation of the elongated equiaxed grain through changing the local temperature gradient and dendritic growth velocity.

One should note that, in our present simulations, dendrite fragmentation is neglected because the magnitude of convection is very small. In the future work, the focus will be on the remelt of dendrite arms, and the effect of dendrite fragmentation on the CET.

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