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Microstructure of aluminum twin-roll casting based on Cellular Automation

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Abstract: Nucleation and growth model based on Cellular Automation(CA) incorporated with macro heat transfer calculation was presented to simulate the microstructure of aluminum twin-roll casting. The dynamics model of dendrite tip (KGT model) was amended in view of characteristics of aluminum twin-roll casting. Through the numerical simulation on solidification structure under different casting speeds, it can be seen that when the casting speed is 1.3 m/min, that is, under conditions of conventional roll casting, coarse columnar grains dominate the solidification structure, and equiaxed grains exist in the center of aluminum strip. When the casting speed continuously increases to 8 m/min, that is, under the conditions of thin-gauge high-speed casting, columnar grains in solidification structure all convert into equiaxed grains. Experimental and numerical results agree well.

Key words: twin-roll casting; aluminum microstructure; Cellular Automation(CA)

1 Introduction

Aluminum twin-roll casting is a new process, which turns liquid aluminum into strip directly. It puts the casting and hot rolling process of traditional aluminum strip into integration, on one hand, to complete continuous cooling and solidification, on the other hand, to produce plastic deformation. It has been widely used for its outstanding advantages, such as simple process, low energy consumption, short production cycle, low cost and low investment.

In the process of aluminum twin-roll casting, the microstructures of materials depend on the casting process parameters, and microstructure has a great impact on its properties. Therefore, to find out the disciplines of microstructure formation in roll casting is an economical and feasible way to optimize the parameters of casting process and to get high quality strip by the calculation and prediction of casting process.

In the recent ten years, many kinds of methods about solidification structure simulation have been presented, which can be summed up in two main categories: deterministic simulation and stochastic simulation. Deterministic simulation, based solidification dynamics, meets the physical background of grain growth, but some random phenomena in the process of grain growth cannot be considered, including the random distribution of grain nuclei, random orientation of the grain and the conversion from columnar grains to equiaxed grains and so on[1-3]. Phase-field model reflects the comprehensive role of the solute diffusion, order and thermodynamic driver. The shape, curvature and movement of solid/liquid interface of metal system can be described with the solution of field equations [4–9], and the metal solidification process can be realistically simulated. However, the computational domain is not large enough for actual roll casting. The two methods including Monte Carlo (called MC) method and Cellular Automation (called CA) are more representative among the stochastic methods. Probability theory is introduced to MC method to deal with the distribution of nucleation position and grain growth orientation at random. Images similar with the actual

metallography can be got by MC method, and the impact different process parameters manifested[10-12]. However, MC simulation lacks physical infrastructure, and the simulation time-step has nothing to do with the actual solidification time. CA law was initially used to simulate the grain growth of recrystallization, and later it was introduced to simulate the formation of the grain in the solidification process by GANDIN and RAPPAZ [13-14]. Based on physical mechanism of the process of nucleation and kinetics of grain growth, the size and distribution of grain can be got, and the formation of columnar grains and the conversion from columnar grains to equiaxed grains can also be described by CA. In recent years, CA model has been used to study the phase transition in solidification process, and it has made a lot of progress[15-23]. Formation law of solidification microstructures in roll casting was studied in the present work by the established mathematical model of nucleation and grain growth based on CA.

2 Mathematical model

2.1 Nucleation model

Continuous nucleation model which was heterogeneous nucleation based on Gaussian distribution was used.

Assume that nucleation occurs at different positions, and these nucleation locations can be described by continuous rather than discrete distribution function, $dn/d(\Delta T)$. The density of grains $n(\Delta T)$ at a given undercooling ΔT is described by the integral of nucleation density distribution:

$$n(\Delta T) = \int_0^{\Delta T} \frac{\mathrm{d}n}{\mathrm{d}(\Delta T')} \,\mathrm{d}(\Delta T') \tag{1}$$

$$\frac{\mathrm{d}n}{\mathrm{d}(\Delta T)} = \frac{n_{\mathrm{max}}}{\sqrt{2\pi}\Delta T_{\mathrm{\sigma}}} \exp\left[\frac{1}{2} \left(\frac{\Delta T' - \Delta T_{\mathrm{N}}}{\Delta T_{\mathrm{\sigma}}}\right)^{2}\right]$$
 (2)

where $\Delta T_{\rm N}$ is the mean nucleation undercooling, $\Delta T_{\rm o}$ is the standard curvature undercooling, and $n_{\rm max}$ is the total density of grains.

2.2 Growth model

In KGT model, undercooling ΔT is composed of four parts:

$$\Delta T = \Delta T_{\rm C} + \Delta T_{\rm R} + \Delta T_{\rm T} + \Delta T_{\rm K} \tag{3}$$

The twin-roll casting process is a sub-rapid solidification with the nature of directional solidification, therefore, the dendrite growth velocity is not very high relatively to rapid solidification; the kinetic coefficient of alloys is great; and the kinetic undercooling of dendrite

tip can be neglected. As the solidification undergoes in the quasi-equilibrium condition, it can be deemed that the balanced distribution coefficient remains unchanged. Therefore, KGT model can be amended. The amended KGT model can be seen from the following equations:

$$\Delta T = \Delta T_{\rm C} + \Delta T_{\rm R} \tag{4}$$

$$R=2\pi[\Gamma/(mG_{\varepsilon}\xi_{c}-G)]^{1/2}$$
(5)

$$\Omega = Iv(Pe) \tag{6}$$

$$v=2DP_e/R \tag{7}$$

$$\Delta T_C = -(c_1^* - c_0)m_1 \tag{8}$$

$$\Delta T_{\gamma} = -\gamma k f(\theta_i) \tag{9}$$

$$f(\theta_i) = \prod_{i=x,y,z} (1 + \gamma_i \cos(\lambda_i \theta_i))$$
(10)

$$\theta_i = \arccos \frac{\left| P_l^* P_s^* \right|}{i_1 - i_s} \tag{11}$$

where ΔT is the undercooling, $\Delta T_{\rm C}$ is the ingredient undercooling, $\Delta T_{\rm R}$ is the curvature undercooling, $\Delta T_{\rm T}$ is the thermal undercooling, $\Delta T_{\rm K}$ is the kinetics undercooling, R is the growing radius of dendrite tip, Ω is the dendrite growth saturation, c_0 is the initial concentration of the alloy, c_l is the solute concentration at the liquid interface, k is the solute partition coefficient, mis the slope of liquidus, Γ is the Gibbs-Thomson coefficient, G_{ε} is the solute concentration gradient in the forefront liquid of dendrite, G is the temperature gradient, Pe is the Peclet number of solute, Iv(Pe) is the Ivantsov function of Peclet number, ξ_c is the function of Peclet number, v is the growth velocity of dendrite tip, D is the diffusion coefficient of the liquid phase, and θ_i is the angle between the largest grain growth direction and x-axis.

3 Numerical simulation

3.1 Mesh division

During the computing, larger mesh was used to simulate the temperature field, and the cell meshes with smaller size were used for simulation of micro nucleation and growth, then the micro cell temperature can be got by interpolation of macro cell temperature in space and time. Obviously, the temperature is influenced by its neighboring macro-cells, and it is in reverse ratio to the distance between the neighboring macro-cell and point a:

$$T_{\rm a} = \sum_{i=1}^{4} l_i^{-1} T_i / \sum_{i=1}^{4} l_i^{-1} \tag{12}$$

where T_a is the temperature of the micro cell a, T_i is the temperature of the neighboring macro cell, and l_i is the

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