

Numerical simulation on directional solidification of Al-Ni-Co alloy based on FEM

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Abstract: The ratio, of the temperature gradient at the solidification front to the solidification rate of solid-liquid interface, plays a large part in columnar grain growth. The transient temperature fields of directional solidification of Al-Ni-Co alloy were studied by employing a finite element method. The temperature gradient at the solidification front and the solidification rate were analyzed for molten steels pouring at different temperatures. The results show that with different initial pouring temperatures, the individual ratio of the temperature gradient at solidification front to the solidification rate soars up in the initial stage of solidification, then varies within $2,000\text{--}6,000\text{ }^{\circ}\text{C}\cdot\text{s}\cdot\text{cm}^{-2}$, and finally goes down rapidly and even tend to be closed to each other when the solidification thickness reaches 5–6 cm. The simulation result is consistent with the practical production which can provide an available reference for process optimization of directional solidified Al-Ni-Co alloy.

Key words: Al-Ni-Co alloy; finite element method; columnar grain; transient temperature field; directional solidification; temperature gradient; solidification rate

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The directional solidification technique is effectively used to control the grain orientation in solidification structure, eliminate transverse grain-boundary, and obtain columnar grain or single grain structure in order to improve longitudinal mechanical property of the materials. Therefore, this technique, since it was first developed, has made great progress and has been widely applied to develop semiconductor, magnetic, and composite materials. Besides, it is an important tool for theoretical research on the solidification process^[1-4].

Usually most Chinese foundries use a high temperature mould in the production of grain-oriented magnetic steel of LNGT72. To obtain columnar grain castings, the mould temperature has to reach about $1,350\text{ }^{\circ}\text{C}$ and the tapping temperature of the molten steel has to be increased correspondingly^[5]. In practical production, some important factors for columnar grain growth, such as the ratio of the temperature gradient at the solidification front to the solidification rate and its change rule, have not been studied until now. In present work a finite element simulation is adopted

to quantitatively analyze the relationship between the ratio of the temperature gradient to the solidification rate and molten steel temperature. The studied results can be applied to optimize the directional solidification process of Al-Ni-Co alloy.

1 Heat transfer model

1.1 Physical model and assumptions

The directional solidification entity model of Al-Ni-Co alloy is shown in Fig. 1. Major geometry parameters of the model are: 0.28 m outer diameter and 0.232 m inner diameter of mould, 0.028 m height of gate and riser, cooling bottom plate of Grade 45 carbon steel of 0.01 m thickness and 6 castings, each $0.04\text{ m} \times 0.025\text{ m} \times 0.072\text{ m}$.

For simplicity, this physical model is dealt with using the following assumptions: (1) The molten steel is filled instantly into the mould and the initial molten steel temperature is uniform; (2) Mass transfer in liquid and solid is neglected; (3) Heat convection is neglected in the molten steel; (4) The initial temperature distribution of the mould is steady, and changes to non-steady state heat conduction after the molten steel is poured into the mould; (5) The bottom cooling condition is treated as uniform cooling with constant heat flux instead of a gradual cooling state.

1.2 Heat transfer governing equation

Based on the law of conservation of energy and Fourier's law of heat conduction, the following differential equation of 3D unsteady state heat conduction is applied to describe the

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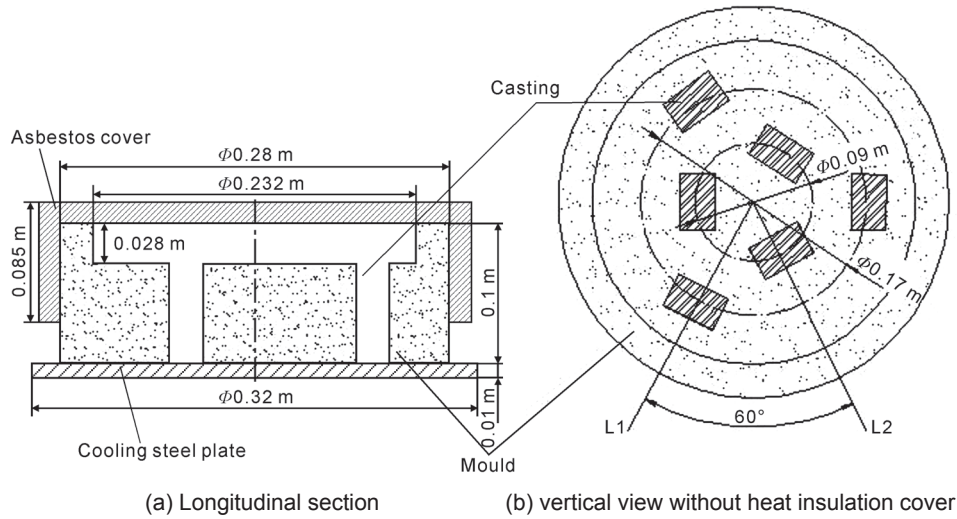


Fig. 1 Schematic diagram of model for directional solidification process

temperature field of conductors:

$$\rho c \frac{\partial T}{\partial \tau} = \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\lambda \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(\lambda \frac{\partial T}{\partial z} \right) + \Phi \quad (1)$$

Where, ρ is density, T is temperature, c is specific heat, Φ is latent heat, τ is time and λ is thermal conductivity; x , y , and z are the coordinate values of some point in the three-dimensional coordinate system.

1.3 Material's parameters and boundary conditions

The model's parameters include thermal conductivity, density, specific heat, enthalpy value, etc. Thermal conductivity, specific heat and enthalpy are non-linear functions of temperature. The enthalpy of the castings has great influence on the crystallization of directional solidification, which will result in major calculation errors if this factor is not considered. Therefore, thermal conductivity, specific heat and enthalpy in this paper are all inputted in temperature-dependent functions.

The top of the mould was treated as being in an adiabatic condition. The bottom of the mould was regarded as having a uniform cooling pattern with a constant heat flux. An effective heat transfer coefficient was introduced to deal with a convective heat exchange with ambient air and radiative heat transfer.

1.4 Phase transition problem during directional solidification

The phase transition during solidification should actually be regarded as a nonlinear transient thermal process. The latent heat in the phase transition is considered in the simulation, which distinguishes it as nonlinear simulation rather than a linear one. Facing this situation, ANSYS incorporates the latent heat during phase transition into the temperature-dependent enthalpy of the materials. At the same time, the time step should be short enough to improve accuracy of the calculation result.

1.5 Mesh division

Due to calculation accuracy and computer hardware conditions, 1/6 simulation domain of 3D entity model ranging from line L1 to line L2 shown in Fig. 1 was selected as a finite element model. The bottom plate was simplified as a cylinder in

establishing the model. Also, ANSYS treats the circumference of the model as a heat insulation, and the asbestos cover on the mould can be regarded as an insulation. The established model did not include the asbestos cover to speed up calculation of the model. This finite element model is shown in Fig. 2.

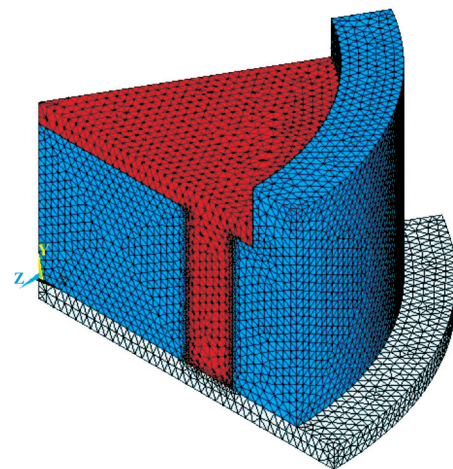


Fig. 2 Finite element model

2 Calculation of temperature gradient and solidification rate

Based on the physical parameters of materials defined above, the relative temperature and heat flux of the mould on corresponding nodes of the established finite element model were used to achieve the initial thermal field for transient temperature calculation through closing the time integral option.

After the initial temperature distribution on the mould was obtained, the transient analysis was processed through updating temperature values on the nodes, opening the time integration option and setting final time.

To obtain the planar solidification structure, the planar interface growth criterion, based on constituent under-cooling theory, is described in the following equation on condition that interaction among solute constituents would not influence their self-diffusion coefficients:^[6]

$$\frac{G_{TL}}{R} \geq -\frac{m_{Lm} w_{c_{0m}} (1-k_{0m})}{k_{0m} D_{mL}} - \frac{m_{Ln} w_{c_{0n}} (1-k_{0n})}{k_{0n} D_{nL}} \quad (2)$$

Where, R is the solidification rate, cm/s; G_{TL} is the temperature gradient at the solidification front, °C/cm; $w_{c_{0m}}$ is the mass fraction of the solute M in liquid, %; $w_{c_{0n}}$ is the mass fraction of the solute N in liquid, %; m_{Lm} is the liquidus slope where $w_{c_{0m}}$ is involved; m_{Ln} is the liquidus slope where $w_{c_{0n}}$ is involved; D_{mL} is M solute atom's self-diffusion coefficient in liquid, cm²/s; D_{nL} is N solute atom's self-diffusion coefficient in liquid, cm²/s; k_{0m} is the equilibrium partition coefficient of the solute M; and k_{0n} is the equilibrium partition coefficient of the solute N.

The right side of Eq. (2) is regarded as constant if the liquid steel flow during solidification is neglected. As a result, controlling solidification rate R and temperature gradient G_{TL} efficiently is beneficial to promoting grain planar interface growth and obtaining good columnar grain structures.

The parameters of R and G_{TL} can be decided by the following equations (3) and (4):

$$R = \frac{D - D_s}{\Delta\tau} \quad (3)$$

$$G_{TL} = \frac{T_L - T}{D_L - D} \quad (4)$$

Where, D , D_s and D_L are a position at the solidification front, the position at the solidification front at the last time point, and the position in liquid, cm, respectively; T is the melting point, °C; T_L is the temperature of some position point in liquid near the solidification front, °C; $\Delta\tau$ is the solidification time interval during the solidification front expansion from last time point to present time point, s.

Based on practical production, the temperature of the bauxite mould was decided to be 1,350 °C, and heat flux was set to be 1.02×10^5 W/m².

3 Results and discussion

Figure 3 illustrates the G_{TL} change curve along the vertical centerline of the castings in the outer ring position of the mould for different initial pouring temperatures. Figure 3 shows that the initial pouring temperature of the molten steel has a great influence on the temperature gradient G_{TL} in liquid at the solidification front in the rapid cooling region. Beyond this rapid cooling region, G_{TL} becomes flat.

Figure 4 shows the solidification rate change with initial pouring temperature of molten steel under the same conditions as Figure 3. Figure 4 shows that the solidification rate decreases with an increase in initial pouring temperature.

Figure 5 shows the variation of G_{TL}/R , the ratio of temperature gradient at the solidification front to the solidification rate along the vertical centerline of the castings, with different pouring temperatures. Figure 5 shows that G_{TL}/R increases rapidly at the initial solidification stage. When the initial pouring temperature is 1,550 °C, G_{TL}/R varies dramatically. G_{TL}/R varies little beyond the rapid cooling region with decrease in initial

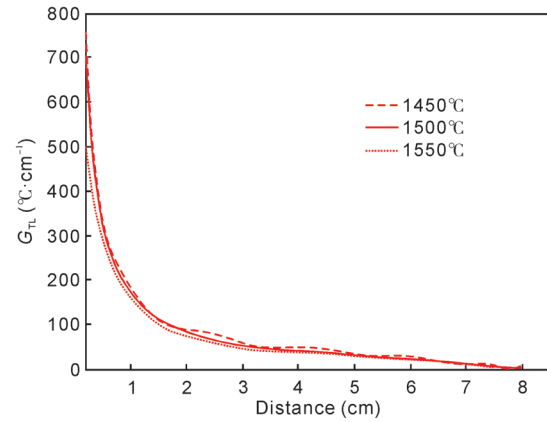


Fig. 3 Effect of pouring temperature on the temperature gradient

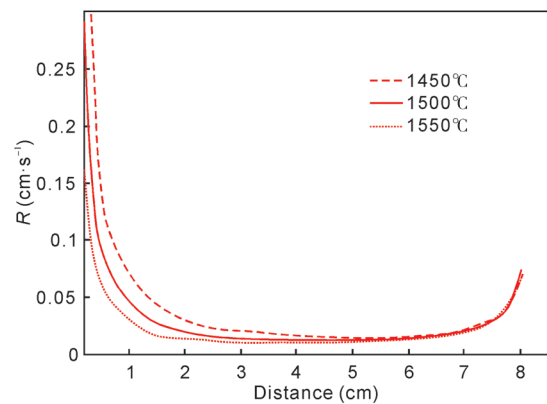


Fig. 4 Effect of pouring temperature on the solidification rate

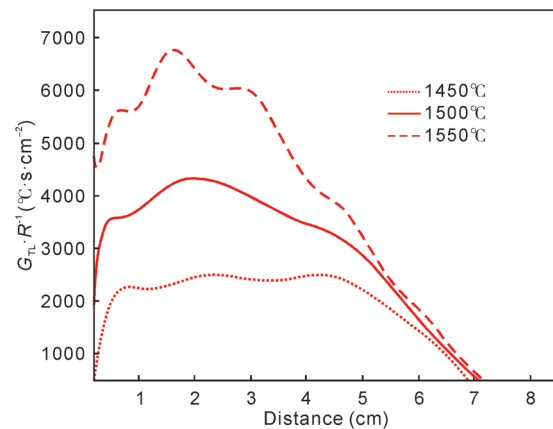


Fig. 5 Effect of pouring temperatures on the ratio of temperature gradient to solidification rate

pouring temperature of molten steel. Finally, G_{TL}/R plunges down and here the G_{TL}/R values are similar for all pouring temperatures.

Figure 6 shows the relationship between the ratio of the temperature gradient to the solidification rate along the vertical centerline of the castings, for different initial pouring temperatures, 1,440, 1,450, and 1,460 °C. Figure 6 shows that, unlike the G_{TL}/R at pouring temperatures of 1,450 and 1,460 °C, the ratio at a pouring temperature of 1,440 °C drops to less than 2000 °C·s·cm⁻² at the vertical distance from the bottom of the casting of 4.7 cm, which results in unfavorable conditions for columnar grain growth.

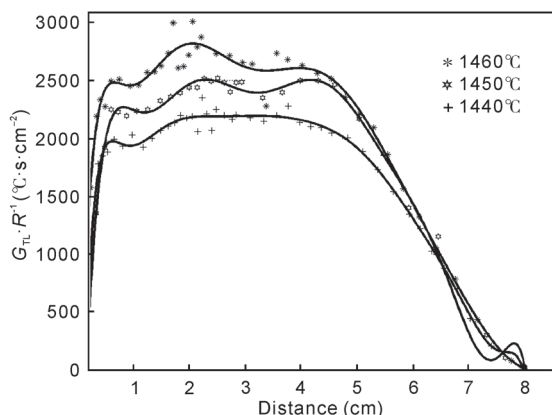
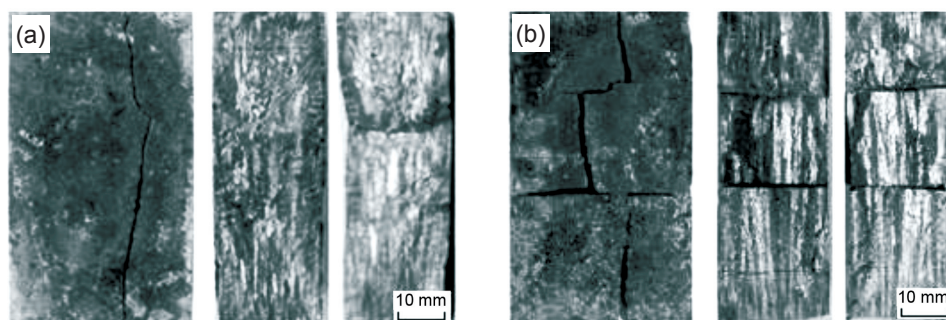


Fig. 6 Effect of pouring temperatures 1,440, 1,450, 1,460°C on the ratio of temperature gradient to solidification rate

In summary, a reasonable increase in the initial pouring temperature of molten steel promotes production of columnar grains because of the increase in the ratio of the temperature gradient to the solidification rate. This results from an increase in the temperature gradient at the solidification front



(a) Tapping temperature at 1,620°C

(b) Tapping temperature at 1,650°C

Fig. 7 Typical castings and columnar grain structure

4 Conclusions

(1) The pouring temperature has a great influence on the solidification rate R , but less effect on the temperature gradient G_{TL} at the solidification front.

(2) With the different pouring temperatures, the ratio of the temperature gradient to the solidification rate first increases dramatically, then this ratio changes within the range 2,000 – 6,000 $^{\circ}\text{C} \cdot \text{s} \cdot \text{cm}^{-2}$, finally this value decreases dramatically, and the ratios for the different temperatures become similar when the solidification thickness reaches 5–6 cm.

(3) Higher pouring temperatures cannot promote columnar grain growth greatly once this columnar grain growth has reached 5–6 cm solidification thickness. In fact, production shows the maximum 6 cm columnar grain length is a limit, whether any increase in mould and tapping temperatures is executed or not. This conclusion verifies the agreement of this simulation and real production results.

(4) The tapping temperature of the molten steel should be controlled between 1,610 $^{\circ}\text{C}$ and 1,650 $^{\circ}\text{C}$.

and a decrease in the solidification rate due to the increase in the initial pouring temperature. But when the columnar grain growth reaches 5–6 cm solidification thickness, G_{TL}/R decreases dramatically, which shows that further increases in the pouring temperature cannot facilitate columnar grain growth greatly.

The castings obtained from production and their columnar grain structures are shown in Fig. 7. It is not easy to produce columnar grains with length over 6 cm through increasing the tapping temperature of the molten steel. The practical production result corresponds with this simulation result. Pouring temperatures over 1,460 $^{\circ}\text{C}$ should be met to obtain columnar grains. This initial pouring temperature depends on the tapping temperature of the molten steel. In practical production the temperature loss is usually about 150 $^{\circ}\text{C}$ during transport of the liquid steel from tapping in the high-frequency induction furnace to pouring into the mould. As a result, the tapping temperature should be 1,610 – 1,650 $^{\circ}\text{C}$. Higher tapping temperatures than this will speed up alloy loss and create more inclusions in the molten steel.

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