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NUMERICAL SIMULATION OF SOLIDIFICATION STRUCTURE OF CONTINUOUSLY CAST BLOOM OF STEEL 20CrNiMo

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A model for predicting solidification structure of continuously cast steel was developed using commercial software ProCAST, and verified by the metallographic examination. Later, the effects of operational parameters on microstructure of continuously cast bloom of alloy steel 20CrNiMo were investigated. The results show that the increase of superheat can promote the columnar grain growth and inhibit the central equiaxed grain growth. When superheat increases from 20 K to 35 K, the central equiaxed grain ratio decreases from 17,8 % to 13,5 %.

Key words: alloyed steel; continuously cast bloom; solidification structure; metallographic examination; numerical simulation

INTRODUCTION

During the continuously cast process, the molten steel is poured into mold through the submerged entry nozzle (SEN), and a great number of nuclei are suddenly formed on the mold surface under the effect of intensive cooling, results in a fine equiaxed zone formed on the strand surface. With the proceed of solidification, some fine grains survive from the competitive growth and grow towards the center. Also, free grains will nucleate in the undercooled melt and successfully block the columnar dendritic growth. Therefore, dendritic growth usually takes place during the solidification of continuously cast steel. Moreover, the solutes are rejected from the dendritic trunk to the interdendritic liquid and redistribute during the dendritic growth process. The complicated dendrite network affects the well mixing of bulk liquid with enriched solute in the mushy zone, which causes the uneven solute distribution over microscopic and macroscopic scales in the cast section [1]. Seriously, if the dendritic overgrowth develops, the mini-ingot will form in the strand due to dendrite bridging and inhibit the effective mixing of molten steel, resulting in severe macrosegregation, shrinkage cavity and porosity. These solidification defects have a great deleterious effect on the mechanical properties of final products [2]. So the fundamental knowledge about the mechanism of dendritic microstructure formation is required to achieve high quality products.

Up to now, Cellular automation method has been successfully used to simulate the solidification structure of continuously cast steel, but comprehensive understanding on the solidification structure evolution and the effects of operational parameters during the continuously cast steel is still far from satisfaction. The main objective of this work is to develop a model for predicting solidification structure of continuously cast steel using commercial software ProCAST, and investigate the effects of superheat on microstructure of continuously cast bloom.

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MODEL DESCRIPTION

Heat transfer model

In the continuously cast process, the solidification and heat transfer of the strand is dependent on the operational conditions, cooling condition, equipment condition, and so on. In order to simplify the heat transfer and solidification of molten steel during the continuously cast process, we assumed a strand slice was born at the meniscus and moved downward with the casting speed. According to the energy conservation, continuously cast process can be described by the two-dimensional differential heat transfer equation.

$$\rho c\frac{\partial T}{\partial t}=\frac{\partial}{\partial y}\left(k_{eff}\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial x}\left(k_{eff}\frac{\partial T}{\partial x}\right)+\rho L\frac{\partial f_s}{\partial t} \quad (1)$$

where T is the temperature, t is the time, ρ is the liquid density, c is the heat capacity, k_{eff} is the effective thermal conductivity, L is the latent heat of fusion, and f_s is the solid fraction.

According to the model assumption, the initial condition is the pouring temperature of molten steel:

$$T = T_c \quad (2)$$

where T_c is the casting temperature.

When the molten steel is poured into the mold, the heat of molten steel is extracted by the cooling water in mold and the heat flux is expressed by

$$q = 2,68 - 0,272\sqrt{t} \quad (3)$$

where q is heat flux, t is the dwell time of molten steel in the mold.

The effective heat transfer coefficient is an important parameter to characterize the heat transfer capability in the secondary cooling zone and mainly depends on the nozzle type, nozzle arrangement, water flow density, water temperature, and strand surface condition, *etc*. According to the previous studies [3], the effective heat transfer coefficient is given by as follows:

$$h = aW^b \quad (4)$$

where h is the effective heat transfer coefficient, W is the water flow density, a and b are empirical parameters, and respectively 610 and 0,395 in the present study.

The heat of stand is mainly removed by the heat radiation in the air cooling zone, which can be converted into convective heat transfer for simplifying the calculation. The equivalent heat transfer coefficient is determined as following:

$$h_e = \varepsilon\sigma(T_s^2 + T_{amb}^2)(T_s + T_{amb}) \quad (5)$$

where h_e is the equivalent heat transfer coefficient, T_s is the strand surface temperature, T_{amb} is the ambient temperature, the Stefan-Boltzmann constant is $\sigma = 5,67 \times 10^{-8}$ W·m^{-2}·K^{-4}, ε is the emissivity.

Nucleation model

A continuous nucleation distribution, dn/d(ΔT), was used to describe the grain density increase, dn, which is induced by an increase in the undercooling, d(ΔT), and given by as followings [4]:

$$\frac{dn}{d(\Delta T)} = \frac{n_{max}}{\sqrt{2\pi}\Delta T_\sigma} \exp\left[-\frac{(\Delta T - \Delta T_n)^2}{2\Delta T_\sigma^2}\right] \quad (6)$$

where ΔT_n is average nucleation undercooling, ΔT_s is the standard deviation, and n_{max} is maximum nuclei density given by the integral of the total distribution (from zero undercooling to infinite undercooling).

Thus, for given undercooling, ΔT, the grain density, n(ΔT), can be determined as follows:

$$n(\Delta T) = \int_0^{\Delta T} \frac{dn}{d(\Delta T)} d(\Delta T) \quad (7)$$

Dendrite tip growth kinetics model

During the solidification of the alloy, the dendritic growth is mainly dependent on the local undercooling. In general, the total undercooling, ΔT, mainly consists of solutal undercooling, ΔT_c, thermal undercooling, ΔT_t, curvature undercooling, ΔT_r, and kinetic undercooling, ΔT_k, and is given as following [5]:

$$\Delta T = \Delta T_c + \Delta T_t + \Delta T_r + \Delta T_k \quad (8)$$

Generally, for the dendritic growth controlled by solute diffusion, ΔT_t, ΔT_r, and ΔT_k are usually negligible, and the growth rate of dendrite tip can be described by the KGT model [6]. According to the marginal stability criterion, we can draw:

$$V^2 \frac{\pi^2\Gamma}{P_C^2 D^2} + V \cdot \frac{mC_0(1-k_0)}{D[1-(1-k_0)I_V(P_C)]} + G = 0 \quad (9)$$

where, V is the dendritic tip growth rate (m·s^{-1}), Γ is the Gibbs-Thomson coefficient, $1,9 \times 10^{-7}$ K · m, P_c is the solutal Peclet number, D is the solute diffusion coefficient, m is the liquidus slope, C_0 is the nominal concentration, k_0 is the partition coefficient, $I_v(P_c)$ is the Ivantsov function, G is the temperature gradient, and set as 0, without considering the thermal effect.

In order to speed up the calculation, the growth velocity of dendrite tip is determined by the polynomial regression equation, and given as following:

$$V(\Delta T) = a_2\Delta T^2 + a_3\Delta T^3 \quad (10)$$

where a_2 and a_3 are the coefficients.

PARAMETERS DEFINITION AND MODEL VALIDATION

Material composition

The alloy structural steel 20CrNiMo is continuously cast with bloom size of 300 mm × 360 mm, and the chemical composition is listed in Table 1.

Table 1 **Chemical composition, Partition coefficient, liquidus slope and solute diffusion coefficient of steel 20CrNiMo**

Element	value / wt%	k_0	m / K / wt-%	D_i / 10^{-9}m^2 / s
C	0,205	0,34	-78	11
Si	0,216	0,52	-7,6	8,5
Mn	0,773	0,78	-4,9	2,4
P	0,0157	0,13	-34,4	4,6
S	0,018	0,035	-38	3,5
Cr	0,505	0,95	-1,3	3,3
Ni	0,432	0,75	-3,9	4,3
Mo	0,251	0,8	-2,8	0,55

Thermophysical parameters

Thermophysical parameter is mainly dependent on phase fraction and temperature of solidifying steel, and has a great effect on the solidification microstructure prediction. The back diffusion model is more reasonable to predict the solidification of most alloys, and adopted in the present study. For the alloy structural steel 20CrNiMo, the calculated liquidus and solidus temperatures are 1 786 K and 1 739 K, respectively.

Nucleation and growth parameters

Nucleation is complicated during the continuously cast process of steel and affected by many factors, such as, steel grade, cooling rate, mold surface condition, *etc*. Therefore, the research on the nucleation parameter of commercial steel is relatively few. Based on our previous study [7], we optimize the reference parameters to make the prediction satisfy with the observation results, and the optimum nucleation parameters for the present study is shown in Table 2.

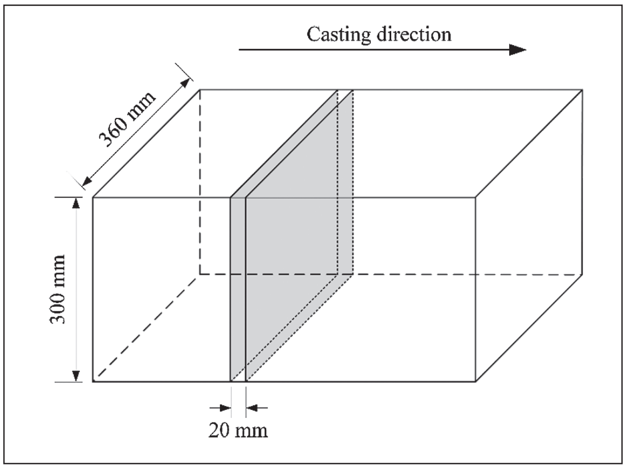

Figure 1 Schematic diagram of sampling details for macrostructure

Table 2 **The parameters of Gauss distribution**

$\Delta T_{s,max}$ / K	$\Delta T_{s,\sigma}$ / K	$n_{s,max}$	$\Delta T_{v,max}$ / K	$\Delta T_{v,\sigma}$ / K	$n_{v,max}$
1,0	0,1	1×10^{8}	1,3	1,6	$1,5\times10^{9}$

The alloy structural steel 20CrNiMo is a commercial multi-component alloy and can be decomposed into several Fe-X pseudo-binary alloy systems for simplifying the calculation. The used phase diagram parameters and solute diffusion coefficients are listed in Table 1. Based on the kinetics model for dendrite tip growth as mentioned above, the kinetics parameters for dendrite tip growth can be determined using the equation (9). Thus, the calculated a_2 and a_3 are respectively 0 and $2,887 \times 10^{-5}$ in equation (10).

Model validation

In order to verify the model, a cross section was cut from the continuously cast bloom of alloy structural steel 20CrNiMo, when the casting condition reaches steady. The casting speed, superheat and secondary cooling intensity for the sampling are respectively 0,5 m / min, 30 K, and 0,23 L / kg. Figure 1 shows the sampling details for experimental measurements. Firstly, one-quarter cross section is macroetched with 1:1 warm hydrochloric acid-water solution to reveal the solidification macrostructure of cast bloom.

Figure 2 shows the experimentally observed and numerically predicted solidification of alloy structural steel 20CrNiMo continuously cast bloom. And the measured and calculated equiaxed grain ratio of bloom are respectively 20,1 % and 20,5 %. The relative error of the equiaxed grain ratio ofbloom between the measurement and calculation is only 1,99 %, which indicates the model accuracy is high enough to predicate the solidification structure of continuously cast steel.

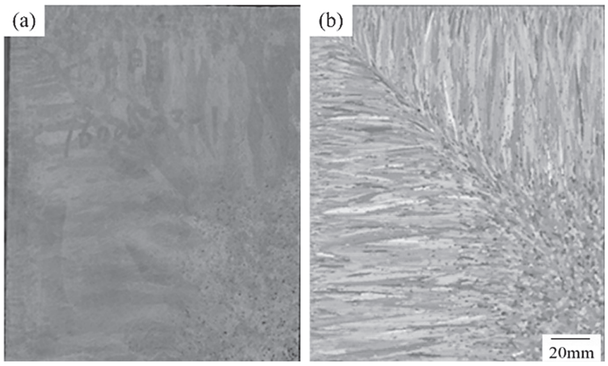

Figure 2 Comparison of experimental observed and simulated solidification structures of steel 20CrNiMo continuously cast bloom: (a) measured, (b) simulated

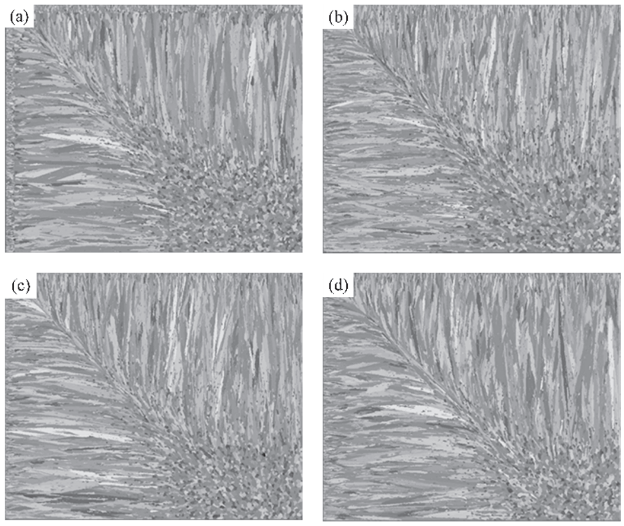

Figure 3 The predicted solidification structure of steel 20CrNiMo continuously cast with different superheats: (a) 20 K, (b) 25 K, (c) 30 K, (d) 35 K

RESULTS AND DISCUSSION

Figure 3 shows the effect of superheat on the solidification structure of continuously cast bloom of alloy structural steel 20CrNiMo. The casting speed and secondary cooling intensity are 0,25 m / min and 0,25 L / kg respectively. It can be seen that with the increase of superheat, both the subsurface chill zone with fine equiaxed grain and central equiaxed grain zone reduce, but the intermediate columnar dendritic grain zone expands. The calculated central equiaxed grain ratio in continuously cast bloom with different superheats is show in Figure 4. It is evident that the central equiaxed grain ratio decreases with the increase of superheat. For the casting condition with different superheats of 20 K, 25 K, 30 K and 35 K, the central equiaxed grain ratios are respectively 17,8 %, 16,2 %, 15,4 %, and 13,5 %. Figure 5 shows effects of superheat on the grain density and average grain area. It is evident that with the increase of superheat from 20 K to 35 K, the grain density decreases from $3,48 \times 10^{5}$ m^{-2} to $2,80 \times 10^{5}$ m^{-2}, but the average grain area increases from $2,87 \times 10^{-6}$ m^{2} to $3,57 \times 10^{-6}$ m^{2}. According to the solidification thermodynamics, these phenomena can be explained that with the increase of superheat, the undercooling at the front of solid/liquid interface decreases and also supercooled interval for nucleation decreases, resulting in nucleation suppression. Consequently, with the increase of super-

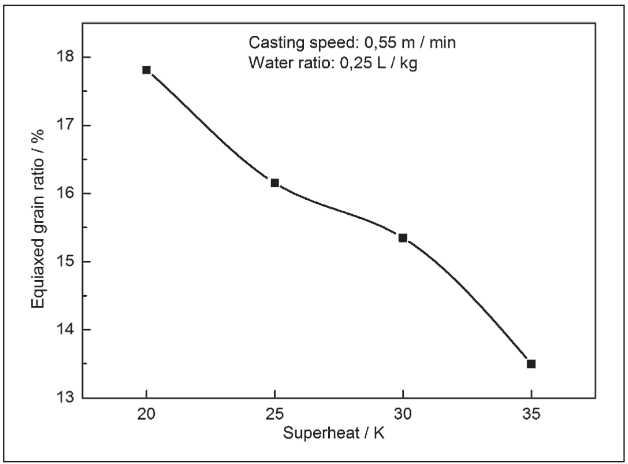

Figure 4 Influence of superheat on central equiaxed grain ratio

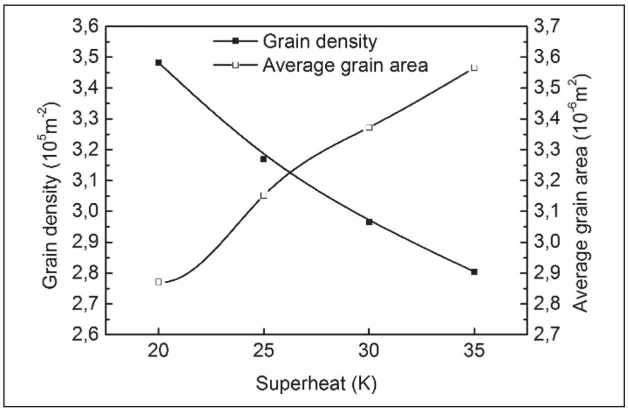

Figure 5 Influence of superheat on the density and average area of grain

heat, the grain density and central equiaxed grain ratio decrease, but the columnar dendrite growth is promoted and becomes coarser.

CONCLUSIONS

In the present study, a model for simulating solidification structure of continuously cast steel was developed using commercial software ProCAST, and validated with the comparison of experimental observation of macrostructure in the continuously cast bloom. The superheat has a great effect on the solidification structure of bloom. With the increase of superheat, the grain nucleation is suppressed, but the columnar dendrite growth is promoted. When superheat increases from 20 K to 35 K, the central equiaxed grain ratio decreases from 17,8 % to 13,5 %, the grain density decreases from $3,48 \times 10^5$ m^{-2} to $2,8 \times 10^5$ m^{-2}, but the average grain area increases from $2,87 \times 10^{-6}$ m^2 to $3,57 \times 10^{-6}$ m^2. This phenomenon is simulated by the present model.

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Note: S. Luo from Northeastern University, Shenyang, China is responsible for English language