The confirmation of simulation parameter and analysis of temperature field of 430 ferrite stainless steel in water-cooling condition with 3D-CAFE method

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Abstract. Under water cooling condition, the solidification structure is almost equiaxed grains, and the diameter of equiaxed grains is 0.5 mm~1mm, columnar grains are relative small, columnar grain width is only a few tenths of millimeters, with the length is 0.5 mm~1.5 mm. When the top heat transfer coefficient is 100 W/ (m^2 K), and the around and the bottom heat transfer coefficient are 2000 W/ (m^2 K)respectively, the solidification structure of the simulation computation is basically with experiment. the casting formed a symmetrical temperature field along the longitudinal section during solidification, the casting top grey area is solidifying contraction.

Introduction

The temperature field have a great influence on the formation of casting solidification structure[1]. Meanwhile, the temperature field influence directly the formation ratio of equiaxed grains in the casting solidification structure[2].The efficient control of temperature field can acquire the necessary solidification structure during solidification of casting[3]. The mass columnar grains have been formed in 430 ferrite stainless steel during solidification which effect its forming property. Minimizing or avoiding the formation of columnar grains and promoting the formation of equiaxed grains is of vital importance to 430 ferrite stainless steel[4,5]. Therefore, it is very significant to research the temperature field during solidification of 430 ferrite stainless steel. In order to analyze the temperature field during casting solidification, the multipoint temperature measuring is necessary, however, it is impossible to achieve in the laboratory, and it is also impossible to analyze the flow field in the laboratory. Numerical simulation can efficiently analyze and research the temperature field and flow field during casting solidification. The 3D-CAFE module of ProCast software to macro-simulate the solidification processuses finite element (FE) method to do simulationcomputation on heat transfer, solute diffusion, momentum transfer as well as other transfer processes during the process of castig solidification[6-8]. FE can calculate the temperature field, solute field and speed field during casting solidification[9].The nucleation and growth of grains can be reproduced by combining FE and CA methods, and the solidification structure under different solidification conditions can be forecasted[10,11]. This paper uses experiment as well as 3D-CAFE module of procast(cellular automaton module together with finite element therefore build up macro-micro module) to analyze the temperature field.

Experimentation and simulation parameters determination

Experimentation results analysis

Vacuum induction furnace was used to smelt 430 ferrite stainless steel with vacuum degree 10Pa; the weight of casting is 5kg, andits main contents in Table 1. As calculated by procast, the solidus andliquidustemperaturewere1733 K and 1771 K, respectively. The metal is casted into the furnace with casting temperature 1821K（The pouring temperature is 1821 K）. The liquid steel filled up into the water-cooled cooper crystallizer(with high purity alumina cover on top)instantly, the bottom and around were water-cooling and top was air-cooling. Attainingacasting which height was 123mm and top diameterwasØ85 mm and bottom diameterwasØ70 mm. The casting wascutted lengthways along its diameter, then polished by sand paper, eroded by $HCl:HNO_3:H_2O=1:1:1$ reagent. The solidification structure of casting is shown in Figure 1(a). The 430 ferrite stainless steel macrostructure is shown in Figure 2. The diameter of equiaxedis0.5 mm~1.5 mm, the closer the casting center equiaxial crystal grain size is smaller. Around the casting there are a little number of columnar grains with relative small size, the width smaller than 1mm, and the length is 0.5 mm~2 mm.

Table1The standard and experimental sample composition of430 ferritic stainless steels (%)

Elements	Cr	C	Si	Mn	S	P
The experimental composition c_o	17	.1	0.44	0.47	0.02	0.03

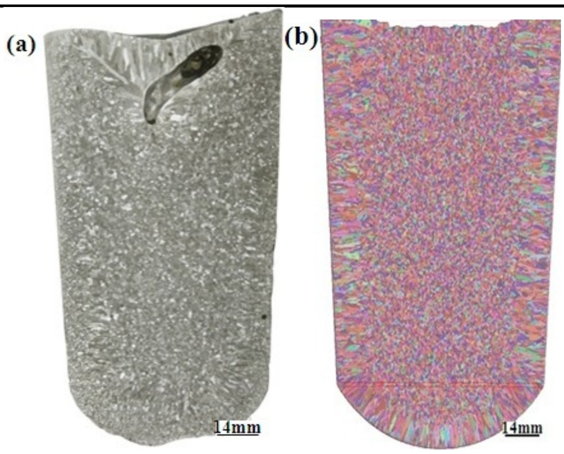

Figure1. The solidification structure of casting（a）experimentation,（b）the simulation computation

（a）

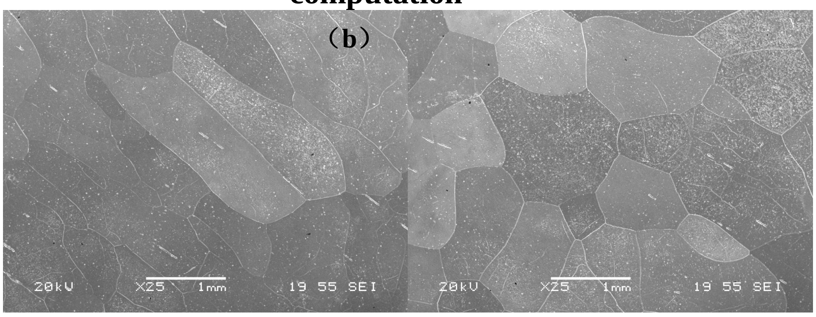

Figure 2. The macrostructure of the castings （a）columnar grains,（b）equiaxed grains

12 Model establishment

(1) Governing equation[12]

Massconservationequation

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u)}{\partial x}+\frac{\partial(\rho v)}{\partial y}+\frac{\partial(\rho w)}{\partial z}=0 \quad (1)$$

Momentum conservation equation

$$\frac{\rho}{f_l}\frac{\partial u}{\partial t}+\frac{\rho}{f_l^2}\left(\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}\right)=$$

$$-\frac{\partial P}{\partial x}+\rho g_x+\frac{\partial}{\partial x}\left(\frac{u}{f_l}\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{u}{f_l}\frac{\partial u}{\partial y}\right)+\frac{\partial}{\partial z}\left(\frac{u}{f_l}\frac{\partial u}{\partial z}\right)-\left(\frac{u}{K}\right)u \quad (2)$$

Energyconservationequation

$$\rho\frac{\partial H}{\partial t}+\rho\frac{\partial H}{\partial T}\left(u\frac{\partial T}{\partial x}+v\frac{\partial T}{\partial y}+w\frac{\partial T}{\partial z}\right)=\frac{\partial}{\partial x}\left(k_T\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k_T\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(k_T\frac{\partial T}{\partial z}\right) \quad (3)$$

which

$H(T) = \int_0^T c_p(T)dT + L(1 - f_s)$(4)

u、v、w are respectively thevelocity component in the direction of x,y,z, m/s; f_l isliquid ratio, %; $f_s$is solid ratio, %; $P$is pressure, Pa; $g_x$is weight component in the direction x, m/s^2; ρ is density, kg/m^3; $u$is absolute viscosity,Pa·s, $k_T$is thermal conductivity, W/(m·K); Kispermeability, m^2; $c_p$is heat capacity, J/kg·K; $t$is time,s; L islatentheatofsolidification, J/kg; T is node temperature vector,K; Hisenthalpy, J/mol.

(2) Heterogeneous nucleation model

3D-CAFE adopts continuous nucleation model,it is assume that heterogeneous nucleation the nucleation appears in different nucleation positions and these nucleation positions can be described by continuous distributionfunction$dn/\mathrm{d}(\Delta T)$,namely Gaussian distribution:

$$\frac{\mathrm{d}n}{\mathrm{d}(\Delta T)} = \frac{n_{max}}{\sqrt{2\pi}\Delta T_\sigma} \exp\left[-\frac{(\Delta T - \Delta T_{max})^2}{2\Delta T_\sigma^2}\right] \quad (5)$$

Where: $\Delta T_{max}$is average nucleation undercooling degree, K; $T_\sigma$isthe standard deviation of nucleati on undercooling degree, K; $n_{max}$is maximal nucleation density integrated from 0 to ∞normal distribut ion, the units of surface nucleation and volume nucleationare m^{-2}and m^{-3},respectively. d$n$increased gra in density caused by increased undercooling degree ΔT, hence the grain density under certain underco oling degree can be calculated by formula (6):

$$n(\Delta T) = \int_0^{\Delta T} \frac{\mathrm{d}n}{\mathrm{d}(\Delta T)} \mathrm{d}(\Delta T) \quad (6)$$

Where:n is grain density.

(3) Kinetic model

In solid-liquid interface front total undercooling degree is:

$$\Delta T = \Delta T_c + \Delta T_t + \Delta T_k + \Delta T_r \quad (7)$$

Where: ΔT_c is constitutional undercooling degree; ΔT_t is heat undercooling degree; ΔT_k is kinetic undercooling degree; ΔT_r is curvature undercooling degree, K. the last three items are very small compared to ΔT_c, hence they are always omitted in calculation process.

In order to accelerate the calculation process, the relation between dendritic growth rate and undercooling degree is fitted using cubic polynomial in the KGT (Kurz-Giovanola-Trivedi) model, the obtained polynomial of dendritic tip growth rate is listed as follows:

$$v = a_2\Delta T^2 + a_3\Delta T^3 \quad (8)$$

Where: a_2 and a_3 are growth kinetics coefficient, m·s^{-1}·K^{-3}

Simulation parameters determination

In order to analyze the temperature field and flow field of 430 ferrite stainless steel during solidification, the 3D-CAFE moudleof procast software is used to conduct simulation computation on casting of the same size. To make the simulated conditions same as the experiment conditions, all around of the simulated calculated casting is heat transferable, and around, top and bottom are used different heat transfer coefficient h. Because the liquidmetal can fill in the water-cooled copper crystallizer instantly, the temperature lost and fluid flow in mold-filling process can be omitted.

With ASTM standard and Figure 2, we can get $n_{v,max}$=1×10^{10} m^{-3}, $n_{s,max}$=3.7×10^7 m^{-2}; other Gaussian distribution parameters are: $\Delta T_{v,max}$=3 K, $\Delta T_{v,\sigma}$=0.5 K, $\Delta T_{s,max}$=2 K, $\Delta T_{s,\sigma}$=0.1 K(in the bulk volume indexed as "v" and at the surface of the mould indexed as "s");the kinetics coefficients for dendritic tip growth are a_2=0, a_3=3×10^{-6} m·s^{-1}·K^{-3}. The mesh parameters of simulation computation are shown in Figure 3, and the thermophysical parametersshown in table 2. When the heat transfer coefficient h=100 W/(m^2 K)(air-cooling), h=2000 W/(m^{2}K)(water-cooling), the solidification structure of casting is shown in Figure 1（b）; asit can see from Figure 1, the solidification structure of simulation computation is basically the same as experimentation, which indicates that the3D-CAFEmoudle of procast software can accurately computate and analyze the 430 ferrite stainless steel.

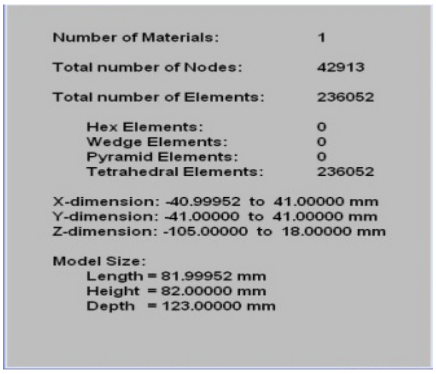

Figure 3. The gridparameters

Table 2.The thermo-physical property parameters

Thermal conductivity (W/m K)	Density ($\times 10^3$Kg/m^3)	Enthalpy ($\times 10^3$KJ/Kg)	Viscosity (Pa.s)	Heat transfer coefficient ($\times 10^3$W/(m^{2}K))
27	7	1.26	7	2

Temperature Results Analysis

The Temperature field means that the temperaturedistributed valueson certain given moments and given coordinate points in heat transfer system. As shown in Figure 4, because the cooling conditions and shape of the casting is symmetrical along the longitudinal section, the casting formed a symmetrical temperature field along the longitudinal section during solidification, the casting top grey area is solidifying contraction. This paper only analyzes half of the temperature field and flow field along the longitudinal section.

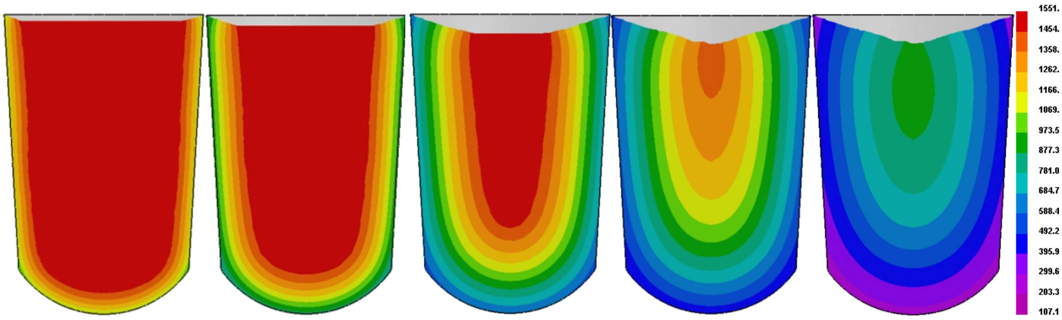

Figure 4.Temperature results-from left to right solidification beginning to ending

Conclusion

(1)Under watercooling condition, the solidification structure of casting is almost equiaxed grains,the proportion of columnar grains is small; the range of equiaxed grain diameter is 0.5 mm~1.5 mm, the more near the casting center, the smaller the equiaxed grain. thereare a little of columnar grains around the casting. These columnar grains are mall with width less than 1mm, and the range of length is 0.5 mm~2 mm.

(2)When the heat transfer coefficient of top h is100 W/(m^2 K)(water cooled), the heat transfer coefficient of around and bottom is 2000 W/(m^2 K)(water cooled), attaining the solidification structure of casting by stimulation computation is similar with experimentation.

(3)The casting formed a symmetrical temperature field along the longitudinal section during solidification, the casting top grey area is solidifying contraction.

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