Numerical Simulation of Solidification Structure Formation in High Mn Steel Casting Using Cellular Automaton Method

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Numerical simulation analysis was carried out to predict the solidification grain structure in commercial scale high Mn steel casting using the cellular automaton (CA) method, and the critical pouring temperature to produce fine equiaxed structure was examined. In the present simulation, heterogeneous nucleation in the molten alloys and the crystal multiplication due to the ‘Big Bang’ mechanism were taken into account. Fine equiaxed grain structure was formed in the simulation with low pouring temperature of 1638 K and mixed structure with columnar and equiaxed crystals was formed with higher pouring temperature of 1663 K. These simulated structures agreed with experimentally observed structures in real castings. To determine the critical pouring temperature to produce fine equiaxed crystal structure, CA simulations for several pouring temperatures were carried out and it was predicted that to obtain fine equiaxed grains in the high Mn steel casting, it will be required to cast with pouring temperature of less than 1648 K.

KEY WORDS: high Mn steel; Big Bang; cellular automaton method; numerical simulation; macrostructure of casting.

1. Introduction

Materials used as the liner of a stone crusher must have high abrasion resistance. High Mn steel casting is one of the liner materials of the stone crusher and has been used for many years as an excellent wear-proof material with ductility. The ability of abrasion resistance of the high Mn steel casting has been improved along with increase in the pressure added during crushing operation. In recent years, with demand for the further improvement of the performance of the stone crusher, longer life time and higher wear-proof characteristic are required to the liner material.

Mechanical properties of the high Mn steel casting are greatly changed depending on the solidification structures such as dendrite morphology and grain size. Especially, the grain size strongly influences the mechanical properties of the casting. Hence, it is expected that very fine grains will improve the abrasion resistance and ductility of a liner material of the stone crusher, because fine grains raise the capability of work hardening of the liner material. Solidified grain structure of the high Mn steel casting is controlled by casting conditions such as alloying elements, pouring temperature, mass of casting, mold size, etc. In those conditions, the increase in the amount of adding elements decreases the ductility of the high Mn steel casting. Hence, the control of pouring temperature is most reliable method to control the solidified grain structure of the high Mn steel casting.

It is well known that fine crystal grains can be obtained by the casting with lower pouring temperature. However, in real casting operation for commercial products, with decrease in the temperature of the molten alloy in a ladle, viscosity of the molten alloy increases and the flowability of the molten alloy decreases, then this makes casting operation difficult. Therefore, some degree of the superheat of the molten alloy in the ladle must be maintained for stable casting operation. Accordingly, it is very important to know the upper limit of the pouring temperature for producing fine grain structure of the casting. However, many experimental works would be required to obtain the optimum pouring temperature of the molten alloy.

In the past two decades, several models for simulating solidification structure formation of alloys during solidification have been developed. Stochastic models such as the Monte Carlo (MC) method1) and cellular automaton (CA) method,2,3) and deterministic models such as phase field (PF) method4–8) have been presented. Many attempts have been carried out to predict solidified structure of alloy castings by using those methods. However, it seems that there were few attempts to predict the solidified structure of commercial casting products prior to real casting operation.

In the present study, we have tried to simulate the solidification grain structure formation process of commercial scale high Mn steel casting using cellular automaton method. The change in solidified grain structure of the casting with change in the pouring temperature of the molten alloy was investigated, and optimum pouring temperature of the molten alloy for obtaining the fine grain structure was examined.
2. Method

2.1. Experiment

The shape of the high Mn steel casting is axial-symmetric and the drawing of a half of the commercial scale casting, runner and sand mold is shown in Fig. 1. Chemical composition of the high Mn steel is shown in Table 1. The two high Mn steel samples of 1.2×10³ kg in mass was melted with an 8 ton electric furnace in the air, and then poured into the sand mold with pouring temperatures of 1 638 K (superheat=40 K) and 1 663 K (superheat=65 K), respectively. The castings were heat treated at 1 423 K for 6h and then quenched into water. After the quenching, the castings were cut at the transverse section, and then etched by using C₂H₅OH–4%HNO₃ reagent and grain macrostructures at the sections were observed.

![Shape of axisymmetric mold and high-manganese steel casting used for the experiment and simulation.](image)

Fig. 1. Shape of axisymmetric mold and high-manganese steel casting used for the experiment and simulation.

| Table 1. Chemical composition of high-manganese steel. (mass%) |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Fe   | C    | Si   | Mn   | P    | S    |
| Bal. | 1.35–1.40 | <0.8 | 20–24 | <0.07 | <0.04 |

2.2. Simulation Model

In the present study, the cellular automaton method (CA) was combined with heat transfer calculation during the solidification process of the high Mn steel casting. Simulation procedure of the CA method is basically the same as that of the CA technique developed by Rappaz and Gandin except for the nucleation model.

2.3. Heat Transfer Calculation

Heat conduction in the casting was calculated by solving the basic heat conduction equation with the form of a cylindrical coordinate:

$$\frac{\partial T}{\partial t} = \frac{\lambda}{\rho C_p} \left( \frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2} \right)$$ (1)

where $\lambda$ is thermal conductivity, $\rho$ is density and $C_p$ is specific heat. The evolution of latent heat during solidification was incorporated into the calculation by using the effective specific heat method as shown in following Eq. (2).

$$C'_p = C_p + L \left( \frac{df}{dt} \right)$$ (2)

where $C'_p$ is effective specific heat, $L$ is latent heat and $f_s$ is the fraction of solid.

Material and thermal properties used in the heat transfer calculation are listed in Table 2.

| Table 2. Materials and thermal properties used in the simulation. |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
|                | High Mn steel   | Sand Mold       | Insulator       | Frame           |
| Thermal Conductivity, $\lambda$ [J/(m·s·K)] | 35.9            | 1.67            | 2.51            | 3.35            |
| Specific Heat, $C_p$ [J/(g·K)]               | 0.867           | 1.05            | 1.05            | 0.628           |
| Density, $\rho$ [Mg/m³]                      | 7.87            | 1.55            | 1.83            | 7.50            |
| Latent Heat, $L$ [J/g]                        | 272.1           | –               | –               | –               |

Heat Transfer Coefficient, $h$ [J/(m²·s·K)]

- Ingot - Mold: 418.6
- Ingot - Insulator: 418.6
- Mold - Insulator: 8372
- Mold - Frame: 10465

Where $\Delta t$ is the time step for numerical calculation, $V_{CA}$
is the area of a CA cell, $\Delta T$ is undercooling, $a$ is maximum undercooling for the nucleation and exponent $n$ regulates the nucleation rate in the simulation and designated as nucleation parameter. It has been demonstrated that the use of the combination of fixed value of $a$, and variable $n$ is effective for the simulation of solidification structure formation.\(^9\) In this nucleation model, the fitting parameter is only the exponent $n$ for the constant value of $a$.

In the present simulation, the effect of the ‘Big Bang’, i.e. copious crystal multiplication at a mold wall during pouring operation was taken into account by the method described in a previous our paper.\(^10\) The amount of crystals formed due to the ‘Big Bang’ was incorporated into the nucleation model as increase in the crystal formation rate in bulk liquid. Total crystal formation rate, $R_{\text{total}}$, was defined as the sum of the contribution of heterogeneous nucleation in bulk liquid, $R_{\text{Nu}}$, and the contribution due to the ‘Big Bang’,

$$R_{\text{total}} = R_{\text{Nu}} + R_{\text{big}} \quad \ldots \ldots (4)$$

The value of $R_{\text{big}}$ was assumed to be independent of the undercooling in melt because the crystals formed at a mold wall were moved by the fluid flow, and the number of free crystals could not be related to the undercooling at the position to which the crystals were carried. Procedure for the formation of a new crystal in undercooled liquid region is as follows. A liquid CA cell is randomly selected based on a random number generated by the program code and if the liquid cell is undercooled state, then the probability for the formation of new crystal was calculated. A random number generated by the program code and if the number is smaller than 0–1 is generated, and if the number is smaller than the probability for the formation of new crystal, then the liquid cell is changed to a solid CA cell. The probability, $p$, for the formation of a new crystal is determined so as to satisfy the total crystal formation rate, $R_{\text{total}}$, shown in the Eq. (4) and expressed as $p = R_{\text{total}} \times \Delta t \times V_{\text{CA}}$.

2.4.2. Growth Kinetics

The KGT (Kurz, Givanoala, Trivedi) model\(^{11,12}\) was used as the model of growth kinetics of a dendrite tip in the high Mn steel. Based on the marginal stability criterion for low pcteclet number, one obtains

$$V^2A + VB + C = 0 \quad \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (5)$$

With

$$A = \frac{\pi^2 \Gamma}{P_r^2 D^2}$$

$$B = \frac{m C_0 (1 - k_b)}{D [1 - (1 - k_b) \nu(P_c)]}$$

$$C = G$$

where $V$ is the growth velocity of a dendrite tip, $\Gamma$ is the Gibbs–Thomson coefficient, $P_c$ is the Peclet number for solute diffusion, $D$ is diffusion coefficient in liquid, $m$ is liquidus slope, $C_0$ is initial concentration, $k_b$ is partition coefficient, $\nu(P_c)$ is the Ivantsov function and $G$ is temperature gradient. For the dendrite growth regime, the imposed temperature gradient, $G$, has little effect on the growth velocity of a dendrite tip and can be regarded as zero.

| Table 3. Material properties used in the calculation of the KGT model. |
|----------------------|----------------------|----------------------|
|                      | Fe-1.35%C           | Fe-20%Mn            |
| Partition Coefficient, $k_b$ | 0.35                | 0.80                |
| Liquidus slope, $m$ [K/mass%] | -70.73              | -3.235              |
| Diffusivity in Liquid, $D$ [m$^2$/s] | 2.0x10$^{-6}$       | 2.0x10$^{-6}$       |
| Gibbs-Thomson Coefficient, $\Gamma$ [mK] | 1.9x10$^{-2}$       | 1.9x10$^{-7}$       |

The undercooling at a tip of dendrite, $\Delta T$, is expressed as follows:

$$\Delta T = m C_0 \left[ \frac{1}{1 - (1 - k_b) \nu(P_c)} \right] + \frac{2 \Gamma}{r} \quad \ldots \ldots (6)$$

where $T_s$ is the melting point of pure Fe and $r$ is the dendrite tip radius. The relationship between the undercooling, $\Delta T$, at the dendrite tip and the growth velocity can be calculated from Eqs. (5) and (6) by substituting an arbitral value of the Peclet number for Eqs. (5) and (6). The material properties used in the calculation are listed in Table 3.

3. Results and Discussion

3.1. Growth Kinetics and Crystal Formation Rate in High Mn Steel

In the present study, the KGT model was used for the growth kinetics of a dendrite tip in the high Mn steel. The KGT model was originally developed for a binary alloy to describe the growth kinetics of a dendrite tip of an alloy. The high Mn steel contains many alloy and impurity elements as shown in Table 1. It was considered that the application of the KGT model to the present simulation with taking account of all contained elements in the high Mn steel is very difficult.

Main alloy elements contained in the high Mn steel are C, Mn and Cr, and it was considered that in those elements, C and Mn elements will influence a growth velocity of a dendrite tip mainly during the solidification of the high Mn steel. Figure 2 shows the relationships between the degree of undercooling and growth velocity of a dendrite tip calculated from the Eqs. (5) and (6) in Fe–1.35wt%C and Fe–20wt%Mn binary alloys.

The material properties used in the calculation are listed in Table 3. Partition coefficient, $k_b$ and liquidus slope, $m$ are estimated from the phase-diagram of Fe–C and Fe–Mn binary alloys. There are a few data for the diffusivity of elements in liquid iron, and a same value\(^{12}\) of $D_c$ for C and Mn is used.

Figure 2(a) shows the case of Fe–1.35wt%C and Fig. 2(b) shows the case of Fe–20wt%Mn and it can be understood that the growth velocity of a dendrite tip of the high Mn steel is mainly governed by C. The difference in the growth velocity shown in the Fig. 2 is ascribed to the difference in the partition coefficient $k_b$ and liquidus slope, $m$. Smaller partition coefficient and larger liquidus slope in the Fe–C system promotes the solute enrichment at the front of a dendrite tip and lower the temperature of a dendrite tip re-
sulting in the decrease in the growth velocity of a dendrite

In the present simulation, the growth velocity of a den-

3.2. Simulated and Observed Structures

In order to solve Eq. (1) numerically, a longitudinal cross
section of the casting was divided into square grids with
5 mm on the r- and z-coordinates and Eq. (1) was converted
into an explicit finite difference equation. In the simulation,
the time step of the numerical calculation was determined
to be 0.5 s by considering the stability of the explicit finite
difference method. The network of CA cells was laid on the
cross section of the casting, and the heat transfer grids were
superimposed on the CA cells. One heat transfer grid con-
tains 100 CA cells, and the size of a CA cell was 0.5 mm

Heat transfer coefficients were evaluated so as to reproduce the measured temperature field in
the solidifying high Mn steel casting by the heat transfer
simulation. Figure 3 shows the measured and simulated
cooling curves in the high Mn steel casting during solidifi-
cation. Simulated cooling curves are good agreement with
those measured in the experiment.

Figure 4 shows simulated solidification macrostructures
in the cross section of the high Mn steel castings composed
of runner, product and riser with pouring temperatures
of 1 638 K (superheat: 40 K) and 1 663 K (superheat: 65 K), respectively. Fine equiaxed grains were formed in
the casting with the lower pouring temperature of 1 638 K.
On the other hand, columnar grains grew up and the column-
lar to equiaxed transition (CET) was occurred in the cast-
ing with the higher pouring temperature of 1 663 K.

Figure 5 shows the comparison between experimentally
observed and simulated solidification macrostructures at
the part of the product in the cross section of the high Mn
steel casting. Almost fine equiaxed structures were ob-
volved in both experimentally observed and simulated
macrostructures for the casting with the lower pouring tem-
perature of 1 638 K.

The upper part of the observed macrostructure shown in
Fig. 5(b) is fine grains and differs from the simulated mac-
rostructure. The upper part of the macrostructure shown in
Fig. 5(b) corresponds to the bottom of the high Mn steel
casting. Therefore, it can be considered that suspended
solids move due to convective flow and gravitational
force resulting in the formation of fine equiaxed grain re-
gion at the bottom of the casting. In the present simulation,
crystals formed in liquid can not move and grow at a fixed
location because the effects of convection and gravitational
force were not taken into account. If the solid movement can be taken into account, a more accurate macrostructure can be simulated.

Average equiaxed grain size observed in the real casting with pouring temperature of 1638 K is about 300 μm or less and this value is finer than that in the simulated macrostructure. This difference was derived from the cell size used in the CA simulation. However it can be said that the present simulation succeeded to reproduce the whole equiaxed grain structure of the casting with lower pouring temperature. When the pouring temperature becomes higher value of 1663 K, columnar crystals grew from mold wall and the CET was occurred in both observed and simulated casting. Hence, it can be predicted that the CET will arise in the grain structures of the casting with pouring temperature between 1638 K and 1663 K.

As described in the Sec. 3.2.1, the crystal multiplication at a mold wall, i.e. ‘Big Bang’ mechanism was introduced in the present simulation. In the ‘Big Bang’ process, copious crystals formed at the mold wall were moved to the center region of a casting due to pouring turbulence or convection and finally an equiaxed region was formed at the inner part of the casting. In the present simulation, to incorporate the effect of the ‘Big Bang’, the total crystal formation rate, \( R_{\text{total}} \), was increased from the heterogeneous nucleation rate in bulk liquid, \( R_{\text{Nu}} \), by the contribution due to the ‘Big Bang’, \( R_{\text{big}} \). Total crystal formation rate, \( R_{\text{total}} \), was defined as the sum of the contribution of heterogeneous nucleation in the liquid, \( R_{\text{Nu}} \), and the contribution due to the Big Bang mechanism, \( R_{\text{big}} \), as shown in Eq. (4). Figure 6 shows the relationship between undercooling and the total crystal formation rate used in the present simulation. A combination of nucleation parameter of \( a=40 \) and \( n=10 \) was used for the heterogeneous nucleation rate in bulk liquid, \( R_{\text{Nu}} \), and the contribution of the ‘Big Bang’ mechanism, \( R_{\text{big}} \), for the casting with pouring temperature of 1638 K. The value of the \( R_{\text{big}} \) was determined by reproducing the macrostructures similar to the experimentally observed macrostructures.

Figure 7 shows the relationship between pouring temperature and the evaluated rate of crystal multiplication, \( R_{\text{big}} \). The \( R_{\text{big}} \) reduces with increase in pouring temperature and this result agrees with the result of our previous study.10)

3.3. Prediction of Solidification Structure

One of the purposes of this study is to know the optimum pouring temperature for obtaining fine equiaxed crystal structure in the commercial scale high Mn steel casting by using the numerical simulation for solidification structure formation. Based on the experimentally observe structures, it was shown that the critical pouring temperature at which the macrostructure of the high Mn steel casting is changed from full equiaxed structure to the mixed structure with equiaxed and columnar crystals exists between 1638 K and 1663 K.

To know the critical pouring temperature for obtaining fine equiaxed structure. Simulation was performed for several pouring temperatures between 1638 K and 1663 K, and the simulated results were shown in Fig. 8. The full equiaxed structure is generated with the pouring temperature of 1648 K or less, and the structure turns out to contain columnar structure when pouring temperature becomes higher than 1653 K. It is presumed that the CET temperature exists between 1648 K and 1653 K. Based on the present simulation, we can know that to obtain fine equiaxed
4. Conclusion

By considering the heterogeneous nucleation rate in bulk liquid and the crystal multiplication due to the ‘Big Bang’ mechanism, the solidification grain structure in commercial scale high Mn steel casting was successfully simulated by using the cellular automaton method. The critical pouring temperature to produce the high Mn steel casting with fine equiaxed grains was estimated to be 1648 K, or less by the present simulation model. It has been demonstrated that the simulation technique used in the present study to predict the solidification grain structure formation is applicable to know the optimum pouring temperature to obtain a real commercial product with fine equiaxed crystals.

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