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Mathematical Model for Growth of Inclusion in Deoxidization on the Basis of Unreacted Core Model

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Abstract: Controlling inclusion composition, from the point of view of thermodynamics, only explains the probability and limit of reaction. However, kinetics makes the nucleation and the velocity of growth of inclusions clear, and these kinetic factors are very important to the quality of slab. The basic kinetic theory of unreacted core model was used to build the mathematical model for the growth of inclusions and the concerned software was developed through Visual Basic 6.0. The time that different radius inclusions attain saturation was calculated to determine the controlling step of reaction between steel and inclusions. The time for the growth of inclusion obtained from the model was in good agreement with the data measured by Japanese Okuyama G, which indicated that the model is reasonable.
Key words: inclusion; finite difference method; kinetic theory; unreacted core model

The purpose of kinetics of metallurgical process is to make the mechanism of reaction clear and find out the influence of granularity, concentration, and temperature on the velocity of reaction. According to that, reasonable measures are applied to advance the reactions[1].

Toward high temperature multiphase reaction, its areas are mostly interfaces among phases. Research methods usually make clear which steps are made of the reaction on the basis of the unreacted core model (UCM). Next, the kinetic formulas (mathematical mode) are established through analyses of experiments and theories.

In deoxidation for steel refining, controlling inclusion composition, from the point of view of thermodynamics, only solves the probability and limit of reaction. To make clear the nucleation and the velocity of growth of inclusion is very important for the quality of slab. Basic kinetic theories are used to establish the mathematical models for the growth of inclusion and concerned software has been developed through VB program.

The time that different radii inclusions attain saturation is calculated to determine the controlling step of reaction between steel and inclusion. These can provide reference for discussing and improving the control of inclusion.

1 Mathematical Model

Deoxidation reaction first creates oxide nucleus A_xO_y; then, oxygen and deoxidizer element D diffuses to the exterior of the oxide A_xO_y, making oxide nucleus growing into inclusions ($ADO_{my/n}$). The deoxidation reaction is shown in Eqn. (1).

$$m(A_xO_y)+n[D]=n(ADO_{my/n})+(mx-n)[A] \quad (1)$$

The reaction between D and inclusions consists of at least three stages.

(1) Step 1: Deoxidizer element D in the molten steel diffuses to the interface of steel and inclusion particle.

(2) Reaction: Deoxidation reaction proceeds at the interface of steel and inclusion particle.

(3) Step 2: Products of reaction diffuse from the interface to the interior of the inclusion.

1.1 Diffusion in the molten steel as the controlling step

It is assumed that the deoxidizer element D diffuses in the inclusions quickly. The distribution of reaction product in inclusion varies at an average. The deoxidizer elements D, which is distributed as

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Fig. 1, is the controlling step in the molten steel. According to the theory of UCM, the rate that the deoxidizer element D in the molten steel diffuses to the interface of steel is calculated through Eqn. (2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{4\pi}{3}R_0 w_{(\mathrm{D})}\rho_s\right]=4\pi R_0^2\frac{D_m\rho_m}{R_0}\left\{w_{[\mathrm{D}]}-\frac{w'_{(\mathrm{D})}}{L}\right\} \quad (2)$$

$$w'_{[\mathrm{D}]}=\frac{w'_{(\mathrm{D})}}{L} \quad (3)$$

where $w_{(\mathrm{D})}$ is the concentration of deoxidizer elements in inclusion; $w_{[\mathrm{D}]}$ is the concentration of deoxidizer elements in the steel; $w'_{(\mathrm{D})}$ is the concentration of deoxidizer elements at the side of inclusion at interface of steel and inclusion particle; $w'_{[\mathrm{D}]}$ is the concentration of deoxidizer elements at the side of steel interface of steel and inclusion particle; t is growth time when diffusing in steel; R_0 is the radius of inclusion; ρ_s is the density of slag; ρ_m is the density of steel; D_m is the diffusion coefficient of deoxidizer elements in the inclusion; and L is equilibrium distribution coefficient of deoxidation element at two side of solid and liquid contact interface.

$$w_{(\mathrm{D})}=w_{[\mathrm{D}]}L\left\{1-\exp\left[-\frac{3D_m\rho_m}{R_0L\rho_s}t\right]\right\} \quad (4)$$

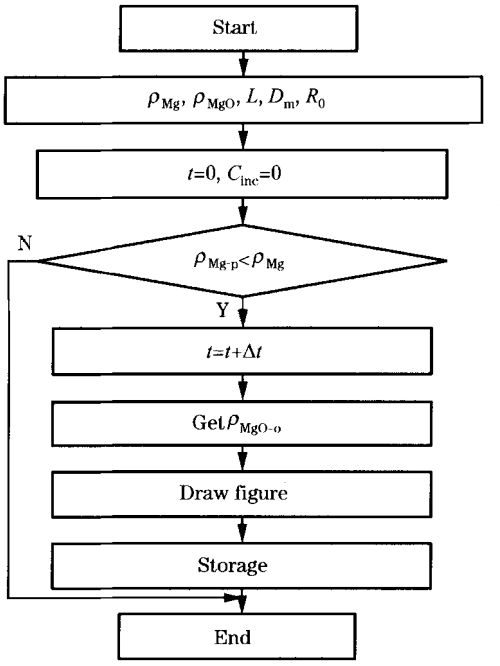
$$w_{(\mathrm{DO}_{my/n})}=\frac{M_\mathrm{D}+\frac{my}{n}M_\mathrm{O}}{M_\mathrm{D}}w_{[\mathrm{D}]}L\left\{1-\exp\left[-\frac{3D_m\rho_m}{R_0L\rho_s}t\right]\right\} \quad (5)$$

where M is molecular mass.

When $w_{[\mathrm{D}]}$ is constant, $w_{(\mathrm{D})}$ can be obtained by Eqn. (4). Eqn. (5) can be deduced according to Eqn. (4). Eqn. (5) can be used to calculate the time taken for the inclusion to grow into saturation concentration of oxidation in inclusion, which can be investigated from system diagram, as shown in Fig. 2.

1.2 Deoxidizer elements in the molten steel layers as the controlling step

As deoxidizer product in the inclusion is the controlling step, concentration of the product is shown in Fig. 3, where $w'_{(\mathrm{DO}_{my/n})}$ is the concentration of deoxidizer product in the inclusion interface between steel and inclusion, and $w^*_{(\mathrm{DO}_{my/n})}$ is the concentration of deoxidizer product at interface of reaction.



ρ_{Mg}—The density of magnesium in steel; ρ_{MgO}—The saturated density of MgO in the computation oxide compound; $\rho_{Mg\text{-}p}$—The density of magnesium after processing; $\rho_{MgO\text{-}o}$—The density of MgO in the computation oxide compound

Fig. 2 Flow chart of program structure

1.2.1 Assumptions

(1) Deoxidizer element D reacts with oxide (A_xO_y), forming ($ADO_{my/n}$);

(2) Particles of inclusion are spherical;

(3) Deoxidizer element D in the molten steel does not change;

(4) Transportation coefficient of the product does not vary from the concentration of product.

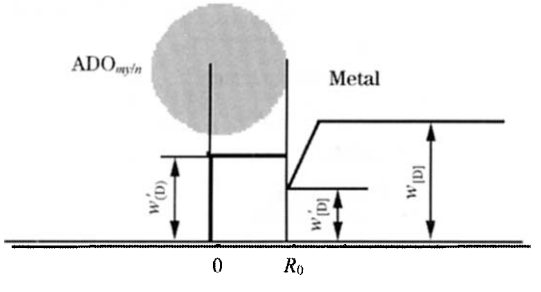


Fig. 1 Diffusion of element D in the molten steel layers as the controlling step

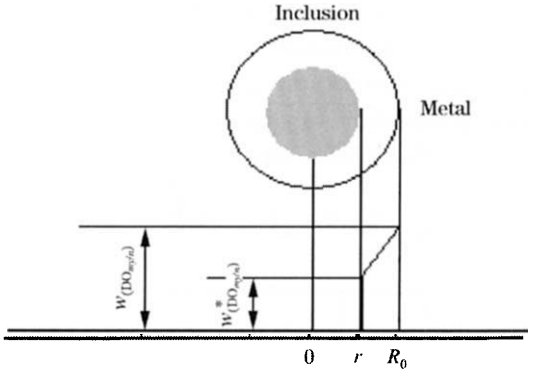


Fig. 3 Diffusion in the inclusion layers as the controlling step