Research Article

Calculation and Analysis of the Structure and Viscosity of \( \text{B}_2\text{O}_3 \)-Regulated \( \text{CaO-Al}_2\text{O}_3 \)-Based Mold Fluxes

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Received 13 September 2020; Revised 9 October 2020; Accepted 16 October 2020; Published 12 November 2020

Academic Editor: Liviu Mitu

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The high content of aluminum in the steel reacts with the \( \text{CaO-SiO}_2 \)-based mold fluxes, resulting in deterioration of the mold slag physical and chemical properties, which cannot be applied to the continuous casting molten slag casting process of high-Mn high-Al steel. Herein, the thermodynamic and structural properties of low-reactivity \( \text{CaO-Al}_2\text{O}_3 \)-based mold fluxes were investigated. The thermodynamic properties were studied based on the first principles of quantum mechanics. The results show that the formation of stable structures of B-O and O-B-O in the mold fluxes was beneficial to reduce the probability of structural interconnection, degree of polymerization, and viscosity of the molten slag. The increase in the ratio of \( \text{CaO/Al}_2\text{O}_3 = 0.88-2 \) led to an increase in the \( \text{O}^{2-} \) concentration. \( \text{O}^{2-} \) entered the \([\text{AlO}_4] \) structure to form a stable structure of \([\text{AlO}_6] \) and \([\text{AlO}_5] \), wherein \([\text{AlO}_6] \) was more stable than \([\text{AlO}_5] \), reducing the degree of polymerization of the network structure. When cosolvent content \( \text{B}_2\text{O}_3 = 2\% - 10\% \), a simple layered structure of \([\text{BO}_3] \) was formed, and the particle migration resistance, break temperature, and viscous activation energy of the mold fluxes were reduced, while the corrected optical basicity of mold fluxes was gradually increased.

1. Introduction

With the rapid industrialization of China, the demand for high value-added steel has gradually increased, especially for high-Mn-high-Al steel. The high-Mn-high-Al steel has excellent mechanics such as great strength, superb plasticity, and low density. This steel is widely used in several fields such as automotive, marine, and nonmagnetic steel [1–7]. The production of high-Mn-high-Al steel uses ingot casting technology. To improve the production efficiency and reduce costs, several steel industries use continuous casting technology in production. The reaction with traditional \( \text{CaO-SiO}_2 \)-based mold fluxes during continuous casting and pouring is as follows:

\[
4[\text{Al}] + 3(\text{SiO}_2) = 2(\text{Al}_2\text{O}_3) + 3[\text{Si}],
\]

\[
2[\text{Mn}] + 3(\text{SiO}_2) = [\text{Si}] + 2(\text{MnO}),
\]

\[
3(\text{MnO}) + 2[\text{Al}] = 2(\text{Al}_2\text{O}_3) + 3[\text{Mn}].
\]

The main component silica in \( \text{CaO-SiO}_2 \)-based mold fluxes reacts with \( \text{Al} \) and \( \text{Mn} \) in high-Mn-high-Al steel as shown in equations (1)–(3). The primary chemical reaction is presented in reaction formula (1). The high aluminum content in high-Mn-high-Al steel is the main reason for the deterioration of physical and chemical properties of traditional \( \text{CaO-SiO}_2 \)-based mold fluxes [8, 9]. When the \( \text{CaO-SiO}_2 \)-based mold flux is in contact with the high-temperature high-Mn-high-Al steel, there is a significant pickup of alumina and dramatic reduction in silica in the spent mold flux. Therefore, the low-reactivity \( \text{CaO-Al}_2\text{O}_3 \)-based mold fluxes are replacing the traditional \( \text{CaO-SiO}_2 \)-based continuous casting mold powder [10–13]. A high amount of \( \text{Al}_2\text{O}_3 \) and low content of \( \text{SiO}_2 \) in low-reactivity \( \text{CaO-Al}_2\text{O}_3 \)-based mold fluxes are expected to lower the driving force for the reaction. Hence, the employment of low-reactivity \( \text{CaO-Al}_2\text{O}_3 \)-based continuous casting mold fluxes can meet the technical requirements of the continuous casting process, ensuring a stable and efficient continuous casting production.
Researchers have conducted a systematic investigation on the physical and chemical properties of molten fluxes [14–16], while some studies [17–20] have been performed on the properties of aluminosilicate molten slag through MD (molecular dynamics) simulation. MD simulations can better analyze the molten slag network structure and associated physical and chemical properties. Wu et al. concluded that, as the content of Al₂O₃ increases, the aluminosilicate network becomes more complex. Also, for a given Al₂O₃ content in different systems, as the electronegativity of the metal cation increases, the disorder of the Al-O structure and network increases, and viscosity decreases. Seo and Tsukihashi used MD simulations to calculate the structural properties of the CaO-Al₂O₃-based molten slag, along with the phase diagram and liquid-phase physicochemical properties of CaO-Al₂O₃-based mold fluxes [23]. Guillot and Sator analyzed the thermodynamic and structural properties of the silicate molten slag under different partial pressures via MD simulations, but due to some limitations in experiments, the properties of the silicate molten slag have not been well studied [24]. The macroscopic characteristics of the continuous casting mold fluxes are determined by the microstructure. In recent years, MD simulations have been widely used to analyze the microstructure of the continuous casting molten slag [25]. Some scholars have focused on the effect of CaO-Al₂O₃-based mold fluxes on the viscosity performance; however, most studies have focused on the impact of flux composition of mold fluxes on the physical and chemical properties. A little attention has been paid to the influence of the CaO/Al₂O₃ ratio on the physical and chemical properties. Al₂O₃-based mold fluxes. Herein, the basic structure and microstructure and macroscopic properties of the CaO-Al₂O₃-based mold fluxes were studied, and the network structure of CaO-Al₂O₃-based mold fluxes was obtained based on molecular dynamics and analyzed with experimental data. The results of this work can provide guidance for the design and optimization of CaO-Al₂O₃-based mold fluxes.

2. Computation Methods

DFT (density functional theory) calculations were performed to compute the structure of the mold fluxes and analyze the thermodynamic properties. The structure was obtained by using the statistical thermodynamics method based on the operating vibration frequency of the optimized structure. The stabilized structure was used as a reactant to explore the transition states via complete linear synchronous transit (LST) and quadratic synchronous transit (QST) methods. The self-consistent field (SCF) method was used with the total energy. The vibrational analysis was used to compute the temperature-dependent enthalpy (H), entropy (S), vibrational free energy (Gᵥ), and constant-pressure heat capacity (Cₚ). The heat capacity (Cₚ) can be given as [29]

\[
C_p = C_{trans} + C_{rot} + C_{vib} = R \sum_i \left( \frac{(hv_i/kT)^2}{[1 - \exp(-hv_i/kT)]^2} + 4R \right).
\]

In formula (4), Ctrans is the translational heat capacity, Crot is the rotational heat capacity, Cᵥ is the vibrational heat capacity, R is the gas constant (8.314 J/mol·K), K is the Boltzmann constant, h is Planck’s constant, T is the absolute temperature, and H is the enthalpy. The enthalpy (H) can be given as

\[
H = H_{vib} + H_{rot} + H_{trans} + RT = \frac{R}{2k} \left( \sum_i hv_i \right).
\]

In formula (5), Htrans is the translational enthalpy, Hrot is the rotational heat enthalpy, and Hᵥ is the vibrational enthalpy. The entropy (S) can be given as

\[
S = S_{trans} + S_{rot} + S_{vib} = 5 \frac{R}{2} \ln T + \frac{5}{2} R \ln \sigma + R \sum_i \left( \frac{\pi}{\sqrt{\sigma}} \frac{8\pi^2 c A}{h} \frac{8\pi^2 c I_b}{h} \frac{8\pi^2 I_c kT^2}{hc} \right) + \frac{3}{2} R
\]

\[
+ R \sum_i \frac{hv_i/kT \exp(-hv_i/kT)}{1 - \exp(-hv_i/kT)} \ln \left[ 1 - \exp(-hv_i/kT) \right].
\]

In formula (6), Strans is the translational entropy, Srot is the rotational entropy, Sᵥ is the vibrational entropy, \( \sigma \) is the pressure, \( \sigma \) is the symmetry number, c is the molar concentration, and \( I_A, I_b, \) and \( I_C \) represent the moment of inertia. \( G_V \) can be given as

\[
G_V = H - T \cdot S,
\]

\[
G = G_V + E(0k),
\]

\[
\Delta G = G_{product} - G_{reaction}.
\]

In formulas (7)–(9), \( G_V \) is the vibrational free energy, \( E(0k) \) is the total energy, \( G_{product} \) is the vibrational free energy product, and \( G_{reaction} \) is the vibrational free energy of the reaction.
3. Analysis of Basic Structure

3.1. Analysis of the Basic Structure. The microstructure of the molten slag determines chemical properties. The stability of the basic network structure is the basis for stable physical and chemical properties of the molten slag. The structural diagram in Figure 1 shows the binding energy of B-O, Si-O, Al-O, Ba-O, Li-O, Ca-O, and Na-O. Binding energy of Si-O is more stable than that of Al-O. The addition of cosolvent SiO2 to mold fluxes will increase the Si-O network structure, increase the stability of the molten slag, and reduce the possibility of interconnection of the molten slag structure, thereby, reducing the degree of polymerization of the mold fluxes. Si-O structure and Al-O structure exist in the mold fluxes in the form of aluminosilicates. With the reduction of the Al-O structure, the mold flux structure reduces the degree of polymerization, degree of polymerization is reduced, and viscosity of the mold flux is lowered. B-O and Si-O structures are more stable than Na-O structures, and B-O and Si-O structures are not easily linked to other structures, which reduces the possibility of interconnection of network structures, makes them easier to form a simple network structure, and reduces the degree of polymerization; therefore, the presence of B-O and Si-O structures reduces the degree of polymerization. For the poorly stable Na-O structure, it is easier to link with other structures to form a complex structure; therefore, the content of Na2O is controlled to reduce the probability of the formation of complex cluster structures. When the content of Na2O is controlled within 12%, the performance of the inner molten slag is stable [30].

In the anionic structure presented in Figure 2, O-B-O is the most stable. Hence, the addition of B2O3 (which aids in the formation of the network) to the molten slag is beneficial for the stability of physical and chemical properties of the mold fluxes, and it also increases the probability of the formation of a [BO3]3− single-layer triangular structure. When the structure is simple, the viscosity of the mold flux is reduced so that the migration energy required by the particles is reduced, and the viscous activation energy is lowered. O-Si-O in the mold flux structure is relatively stable; therefore, O-Si-O in the mold fluxes helps to reduce the probability of structural interconnection. As the ratio of CaO/Al2O3 rises and CaO increases, the free Ca2+ and O2− ions released by CaO can break the combination of the Al-O-Al network structure and form a stable structure Ca-O-Al, and the structure depolymerizes into a simple structure. As presented in Figures 1 and 2, Li-O and O-Li-O have poor stability, and excessive addition of Li2O leads to unstable mold flux viscosity and crystalline properties. Liu et al. [31] found that, in the mold fluxes with high Li2O content, the crystallization rate is clearly increased.

The results of Sun et al. showed that the 27Al MAS-NMR spectra demonstrated three structural units of Al atoms, namely, [AlO₄], [AlO₃], and [AlO₆], which mainly existed in the networks [32]. As shown in Figure 3, [AlO₆] is more stable than [AlO₃] and [AlO₄] is a network modifier. When the CaO/Al2O3 ratio is increased, the main function of CaO is to release O2− and destroy the structure of [AlO₆] aluminosilicate, reduce the degree of aggregation of the network structure, and weaken the mutual links in the structure. As the structure formation of [AlO₆] or [AlO₄] increases, [AlO₃] has a stable octahedral structure, demonstrating a layered isolated distribution, decreased viscosity, increased tendency of random movement of structural units, and reduced resistance to free migration of particles.

There are three coordination numbers in mold flux aluminate: [AlO₄]5−, [AlO₅]7−, and [AlO₆]9−; their structural conversion causes the instability of the aluminate structure and interlinked structure to become complex and poorly stable. The mechanism of action in the molten slag has not yet been established, and hence, it is of great significance to study the aluminate structure of low-reactivity CaO-Al2O3-based mold fluxes. The O2− content in the molten slag is increased to form an octahedral [AlO₆] stable structure. There are more octahedrons in slag structure [AlO₆], which are beneficial for the stability of physical and chemical properties of the molten slag. Figure 4 shows the change in ΔG of different structures with respect to temperature. The reaction that produces a tetrahedral [AlO₄] structure has the greatest ΔG trend, while the reaction that produces [AlO₃] and [AlO₆] structures has lesser ΔG tendency; therefore, it is easier to generate the [AlO₄] structure in the mold fluxes. As the [AlO₃] structure is easier to form, the molten slag forms a tetrahedral [AlO₄] structure which is not as stable as an octahedral structure [AlO₆]. The [AlO₄] increase in the structure is one of the main reasons for the increase in the viscosity of mold fluxes. The network structure [AlO₄] can reduce the tendency of irregular movement in the structure; the free migration resistance and shear force on particles increase, which is also one of the main factors for the increase in viscosity.

4. Sample Preparation and Viscosity Measurement

The chemical composition of the mold fluxes used in this study is listed in Table 1. The chemical reagents used were all pure reagents (>95.5%). CaO was calcined at 800°C in a muffle furnace for 8 h, and other powders were placed at 500°C, as shown in the schematic diagram of the rotary viscometer in Figure 5. A sample of 120 g mold flux was placed in a high-purity graphite crucible, and the viscosity of the molten slag was measured using the rotary viscometer. The Pt/Rh thermocouple was placed directly below the bottom of the high-purity graphite crucible, and castor oil of known viscosity was used for the calibration measurements at room temperature. The heat furnace had the temperature of 1400°C, which was maintained for 8 min to stabilize under argon atmosphere (flow rate: 0.3 L/min). The purpose was to homogenize the temperature and molten slag. The Mo spindle rotated at a fixed speed of 15 r/min; when the signal
from the rotary viscometer stabilized, the furnace was cooled at a rate of 5°C/min, and the viscosity measurements were continued.

5. Results and Discussion

5.1. Effect of the CaO/Al₂O₃ Ratio on Flux Viscosity. Increasing the ratio of CaO/Al₂O₃ in the mold fluxes tends to increase the concentration of free oxygen. The [AlO₅] tetrahedral structure depolymerized into simple and stable structure [AlO₆], the probability of structural interconnection was reduced, and the viscosity of the molten slag decreased. As shown in Figure 6, the mold flux samples A1, A2, A3, and A4 structure fractured with the increase in temperature. When the B₂O₃ content was 2% to 10%, the viscosity of the mold fluxes gradually decreased, and the break temperature of the molten slag was reduced from 1193°C to 1108°C. With the increase in the CaO/Al₂O₃ ratio, cosolvent B₂O₃ mainly existed in a simple two-dimensional [BO₃] structure, and the degree of polymerization of mold fluxes decreased. As a result, the resistance to free migration of particles and the shear force were gradually reduced, the structure was depolymerized, and the viscosity was decreased.

As shown in Figure 7, when \( \omega (\text{CaO})/\omega (\text{Al}_2\text{O}_3) = 0.88–2 \), the viscosity of the mold flux and the degree of aggregation in the network structure were reduced. To lower the reactivity of aluminum in the high-Mn-high-Al steel and
SiO₂ in the mold fluxes, the Al₂O₃ content was increased in the mold fluxes. The aluminate molten slag viscosity is inseparable from the microstructure. When the ratio of CaO/Al₂O₃ was increased, the content of CaO in the mold fluxes increased. As a result, the content of Ca²⁺ ions increased and destroyed the aluminate melt structure. The basic structure O-Al-O was transformed into a stable structure Ca-Al-O; however, excessive addition of CaO or Al₂O₃ can weaken this effect. The high-coordination structure with the high content of Al₂O₃ in the mold fluxes can easily form a complex structure; therefore, the viscous flow mechanism of the coordination structure with different contents of Al₂O₃ was different. As shown in schematic diagrams in Figure 8, [AlO₆] and [AlO₅] generated higher average coordination structures. The main function of CaO was to release O²⁻ to destroy the aluminate structure and form a high-coordination structure, reduce the particle migration resistance and shear force, and lower the viscosity.

As shown in Figure 1, the B-O structure is the most stable in the system; therefore, the addition of cosolvent B₂O₃ to the mold fluxes is beneficial to stabilize the structure and performance. Figure 9 shows the schematic of the generation of B-O three-coordination structure and B-O four-coordination structure. B ions in the molten slag can replace Al in the Al-O coordination structure and form [BO₃]-layered structure and [BO₄] coordination structure. The molten slag structure changed from the [AlO₄] frame structure to the [BO₃]-layered structure, the structure became more relaxed, and the structure changed from complex to simple. The B-O coordination structure increases to increase the fluidity and stability of the molten slag. CaO in the mold fluxes easily released free oxygen and combined with B₂O₃ to form a triangular structure [BO₃], the whole structure became simple, and the resistance of viscosity reduced. Figure 10 shows the schematic diagram for the changes in the network. CaO provides O²⁻ for the depolymerization of complex structures, dissociates the complex structure, and forms a simple and stable structure.

5.2. Viscous Flow Activation Energy and Corrected Optical Basicity. The molten slag temperature was higher than the break temperature, and the molten slag can be considered as a Newtonian fluid. Hence, the change of molten slag viscosity with temperature follows the Arrhenius equation:

$$\eta = A \exp\left(\frac{E_a}{RT}\right),$$

$$\ln \eta = \frac{E_a}{RT} + \ln A,$$

where \(T\) represents the absolute temperature, K; \(A\) is a constant; \(E_a\) is the viscous flow activation energy, kJ/mol;
and \( R \) is the ideal gas constant, 8.314 J/mol·K. The viscous flow activation energy can be calculated using formulas (10) and (11). Figure 11 shows the linear relationship between \( \ln \eta \) and \( 1/T \) in order to calculate the viscous flow activation energy. Figure 11 displays plots of \( \ln \eta \) versus \( T^{-1} \) for fluxes.
with different CaO/Al₂O₃ ratios. The molten slag is in a completely liquid state and is a Newtonian fluid, and the activation energy can be estimated using the Arrhenius equation. Table 2 shows the melting temperature (Tₘ), break temperature (Tₜₜ), and viscous activation energy of experimental slags. As the CaO/Al₂O₃ ratio increased, the viscous flow activation energy and break temperature decreased, which were higher than those reported by Zhiron et al. [33]. The main reason is that the cosolvent was different in the experimental research of mold fluxes. Also, other research works have reported different mold flux network structures resulting in different viscous activation energies. As the ratio of CaO/Al₂O₃ increased, the shear force on particles in free motion decreased, the ability of particles to move freely reduced, and the activation energy and viscosity decreased. These results are consistent with the law of activation energy and viscosity in the traditional mold fluxes.

$$\Lambda_{corr} = \frac{\sum(X_1 n_1 \Lambda + X_2 n_2 \Lambda + X_3 n_3 \Lambda + X_4 n_4 \Lambda \cdots)}{\sum(X_1 n_1 + X_2 n_2 + X_3 n_3 + X_4 n_4 \cdots)}.$$  \hspace{1cm} (12)

The optical basicity (Λ) characterizes the ‘availability’ of providing free oxygen ions, which indicates the degree of polymerization of the melts. A corrected optical basicity ($\Lambda_{corr}$) was proposed by Mills to charge-balance the Al³⁺ ions incorporated into the Si⁴⁺ chain or ring [34]. In formula (12), Λ is the optical basicity, X is the mole fraction, n is the number of slag oxygen atoms in the component molecule, and $\Lambda_{corr}$ is the corrected optical basicity.

The $\Lambda_{corr}$ values of mold powders A1 to A4 are listed in Table 2. From A1 to A4, $\Lambda_{corr}$ of the mold powder increased, and the viscosity decreased. As the ratio of CaO/Al₂O₃ increased from 0.88 to 2, the break temperature and activation energy decreased. These results are consistent with the law of alkalinity and viscosity in the traditional mold fluxes.

5.3. Effect of the Structure on Flux Viscosity. When the CaO/Al₂O₃ ratio varied from 0.88 to 2 in mold fluxes, the increase in the content of CaO increased the number of Ca⁺ ions to compensate for the corresponding anions in the mold fluxes, forming stable structure Ca-O-Al and reducing the probability of interconnection of the molten slag structure. In the mold flux structure, Al-O and [AlO₄] have low structural stability, and mold fluxes tend to increase the probability of the complex structure. As the content of Al₂O₃ in the mold fluxes increased, the main aluminate structure [AlO₄] was gradually formed. Theoretically, it can be considered that all Al³⁺ existed in the form of [AlO₄], and Al₂O₃ continuously replaced SiO₂ in the mold fluxes. The stable [SiO₄] structure decreased and the unstable [AlO₄] structure increased, and the probability of network interconnection increased. The continuous addition of O²⁻ to aluminate can promote the formation of a more stable structure of the tetrahedral aluminate unit network (Figure 3). The chemical reaction $\Delta G$ tends to generate aluminate unstable structure [AlO₂]. As the CaO/Al₂O₃ ratio increased, the content of O²⁻ ions increased. The [AlO₆] octahedral structure increased, and the [AlO₄] tetrahedral structure was reduced, which shows that the network structure was reformed, and the viscosity was reduced. The mold fluxes were mainly composed of the [AlO₆] octahedral structure, suggesting that the network structure was reformed, and the viscosity was reduced. The [AlO₄] structure is not conducive to the interconnection of the network structure. Figure 12 shows the
mold flux structure changed from the original Al-O structure to \([\text{AlO}_4]\), \([\text{AlO}_5]\), and \([\text{AlO}_6]\) structures. In the mold fluxes, the network structure is related to the relative displacement and the connection mode. At first, the microstructure of mold fluxes was investigated as the basic structure is directly related to the viscosity of the mold fluxes. Figure 2 shows the anion structure; the cation in the mold fluxes connects the anion structure through the bridge oxygen bond. The network structure changed from simple to a complex structure, and the complex structures needed to overcome viscous resistance. Another reason for the change in molten slag viscosity is temperature. The increase in temperature led to a decrease in the force between ions and depolymerized bridging oxygen in the melt into nonbridging oxygen. The particle ion migration is easier when the temperature rises, and the viscous resistance decreases. With the addition of cosolvent \(\text{B}_2\text{O}_3\) to the mold fluxes, the metal oxide formed a low-melting eutectic compound, thereby, reducing the viscosity of the mold flux system. \(\text{B}^{3+}\) mainly forms the \([\text{BO}_3]\) structural unit in this mold flux system, and the \([\text{BO}_3]\) structural unit forms a two-dimensional, single-layer simple structure. In this slag system, several factors compete with each other and, ultimately, affect the viscosity of the slag system.

6. Conclusions

Herein, the variations of the structure and viscosity of CaO-Al\(_2\)O\(_3\)-based mold fluxes were investigated. The following conclusions can be made:

(1) B-O is more stable than Na-O, and B-O is not easily linked to other structures, relatively weakening the mold flux structure and lowering the degree of polymerization. For the Na-O structure with poor stability, it is easy to link with other structures to form a complex structure.

(2) The reaction to form a tetrahedral \([\text{AlO}_4]\) structure has the largest \(\Delta G\) trend, while the reaction to form \([\text{AlO}_5]\) and \([\text{AlO}_6]\) structures has a lower \(\Delta G\) trend. Therefore, the \([\text{AlO}_4]\) structure is more likely to exist in the slag, and the octahedral \([\text{AlO}_6]\) structure is stable; increasing the stable \([\text{AlO}_6]\) structure is not conducive for the network structure connections, and the network structure is depolymerized.

(3) When the content of \(\text{B}_2\text{O}_3\) is 2%–10%, it is easier for CaO to release free oxygen in the mold fluxes and combine with \(\text{B}_2\text{O}_3\) to form a triangular structure \([\text{BO}_3]\); single-layer \([\text{BO}_3]\) has a simple and stable structure, reducing the possibility of forming a complex structure. When CaO/Al\(_2\)O\(_3\) 0.88–2, the viscosity and break temperature gradually decrease, and the particle migration resistance decreases.

Data Availability

All the data generated or analyzed during this study are included within the article.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

Acknowledgments

The authors are grateful for the financial support provided by National Key R&D Project of China (no. 2017YFC0805100) and Science and Technology Projects of Liaoning Province (no. 2018307003). The project (no. 2017-01-04) was supported by the State Key Laboratory of Metallic Materials for Offshore Equipment and Applications.
References

[1] I. Gutierrez-Urrutia and D. Raabe, “Multistage strain hardening through dislocation substructure and twinning in a high strength and ductile weight-reduced Fe-Mn-Al-C steel,” Acta Materialia, vol. 60, no. 16, pp. 5791–5802, 2012.

[2] J. D. Yoo and K. Park, “Microband-induced plasticity in a high Mn-Al-C light steel,” Materials Science and Engineering A-Structural Materials Properties Microstructure and Processing, vol. 34, pp. 417–424, 2008.

[3] J. Gao, G. Wen, T. Huang, B. Bai, P. Tang, and Q. Liu, “Effect of slag-streak reaction on the structure and viscosity of CaO-SiO2-based mold flux during high-Al steel casting,” Journal of Non-crystalline Solids, vol. 452, pp. 119–124, 2016.

[4] S. E. Kang, A. Tuling, I. Lau, J. R. Banerjee, and B. Mintz, “The hot ductility of Nb/V containing high Al, TWIP steels,” Materials Science and Technology, vol. 27, no. 5, pp. 909–915, 2013.

[5] A. S. Hamada, L. P. Karjalainen, and M. C. Somani, “Constitutive behaviour of high-Mn-Al twip steels at hot rolling temperatures,” Canadian Metallurgical Quarterly, vol. 46, no. 1, pp. 47–56, 2014.

[6] R. M. Skolky and E. I. Poliaik, “Aspects of production hot rolling of Nb microalloyed high Al high strength steels,” Materials Science Forum, vol. 500, pp. 187–194, 2005.

[7] C. xj_horning and S. Sridhar, “Grainboundaryridgeformation during initial high temperature oxidation of Mn/Al TRIP steel,” Philosophical Magazine, vol. 87, no. 23, pp. 3479–3499, 2007.

[8] M. S. Kim, M. S. Park, and Y. B. Kang, “A reaction between high Mn-high Al steel and CaO-SiO2-type molten mold flux: reduction of additive oxide components in mold flux by Al in steel,” Metallurgical and Materials Transactions B, vol. 50, no. 5, pp. 2077–2082, 2019.

[9] J. Yang, D. Chen, M. Long, and H. Duan, “An approach for modelling slag infiltration and heat transfer in continuous casting mold for high Mn-high Al steel,” Metals-Open Access Metallurgy Journal, vol. 10, no. 1, pp. 51–59, 2019.

[10] C. B. Shi, M. D. Seo, J. W. Cho, and S. H. Kim, “Crystallization characteristics of CaO-Al2O3-based mold flux and their effects on in-mold performance during high-aluminum TRIP steels continuous casting,” Metallurgical and Materials Transactions A, vol. 45, no. 3, pp. 1081–1097, 2014.

[11] X. Dan, W. Wanlin, and L. Boxun, “Effects of B2O3 and BaO on the crystallization behavior of CaO-Al2O3-based mold flux for casting high-Al steels,” Metallurgical and Materials Transactions B and Materials Processing Science, vol. 46, no. 2, pp. 1–9, 2015.

[12] J. Li, B. Kong, L. Jiang et al., “Effect of B2O3 on slag-metal reaction between CaO-Al2O3-based mold flux and high aluminum steel,” High Temperature Materials and Processes, vol. 37, no. 9–10, pp. 981–985, 2018.

[13] P. Yan, S. Huang, L. Pandelaers, J. Van Dyck, M. Guo, and B. Blanpain, “Effect of the CaO-Al2O3-based top slag on the cleanliness of stainless steel during secondary metallurgy,” Metallurgical and Materials Transactions B, vol. 44, no. 5, pp. 1105–1119, 2013.

[14] Y. Xiong, W. Guanghua, T. Ping et al., “Research progress in crystallizing properties of mold flux for continuous casting,” Materials Review, vol. 24, no. 5, pp. 101–105, 2010.

[15] X. Zhang, T. Jiang, X. Xue, B. Xue, and B. Hu, “Influence of MgO/Al2O3Ratio on viscosity of blast furnace slag with high Al2O3Content,” Steel Research International, vol. 87, no. 1, pp. 87–94, 2016.

[16] X. H. Zhu, L. G. Zhu, Y. Liu and P. F. Wang, “Effect of basicity on continuous casting mold flux properties”, Advanced Materials Research, vol. 567, no. 6, pp. 62–65, 2012.

[17] S. S. Jung, G. H. Kim, I. Sohn, G. H. Kim, and I. Sohn, “Thermophysical properties of continuous casting mold flux for advanced steel developments,” Transactions of the Indian Institute of Metals, vol. 66, no. 5-6, pp. 577–585, 2013.

[18] W. Xinguan, J. Hebin, and Z. Liguang, “Effect of B2O3 on properties and structure of CaO-Al2O3-SiO2 continuous casting mold flux,” Materials Reports, vol. 66, 2019.

[19] T. Wu, Q. Wang, T. Yao, Q. Wang, T. Yao, and S. He, “Molecular dynamics simulations of the structural properties of Al2O3-based binary systems,” Journal of Non-crystalline Solids, vol. 435, pp. 17–26, 2016.

[20] B. R. Gel’chinskii, E. V. Dyul’dina, and L. I. Leont’ev, “Molecular-dynamic simulation of the melt of an industrial oxide–fluoride mold flux,” Steel in Translation, vol. 49, no. 9, pp. 601–605, 2019.

[21] T. Wu, S. He, Y. He, Y. Liang, and Q. Wang, “Molecular dynamics simulation of the structure and properties for the CaO-SiO2 and CaO-Al2O3 systems,” Journal of Non-crystalline Solids, vol. 411, pp. 145–151, 2015.

[22] W. Ting, Q. Wang, and Y. Chengfeng, “Structural and viscosity properties of CaO-SiO2-Al2O3-FeO slags based on molecular dynamic simulation,” Glass-Ceramics and Glassy Composites, vol. 450, pp. 23–31, 2016.

[23] W. G. Seo and F. Tsukihashi, “Molecular dynamics simulation of the thermodynamic and structural properties for the CaO-SiO2 system,” ISIJ International, vol. 44, no. 11, pp. 1817–1825, 2004.

[24] B. Guillot and N. Sator, “A computer simulation study of natural silicate melts. Part II: high pressure properties,” Geochimica et Cosmochimica Acta, vol. 71, no. 18, pp. 4538–4556, 2007.

[25] D. K. Belashchenko, “Computer simulation of the structure and properties of non-crystalline oxides,” Russian Chemical Reviews, vol. 66, no. 9, pp. 733–762, 1997.

[26] A. B. Belonosshko and L. S. Dubrovinsky, “Molecular and lattice dynamics study of the MgO-SiO2 system using a transferable interatomic potential,” Geochimica et Cosmochimica Acta, vol. 60, no. 10, pp. 1645–1656, 1996.

[27] L. Forsbacka, L. Holappa, A. Kondratiev, and E. Jak, “Experimental study and modelling of viscosity of chromium containing slags,” Steel Research International, vol. 78, no. 9, pp. 676–684, 2007.

[28] G. H. Zhang, K. C. Chou, and K. Mills, “Modelling viscosities of CaO-MgO-Al2O3-SiO2 molten slags,” ISIJ International, vol. 52, no. 3, pp. 355–362, 2012.

[29] J. Sanchez, H. Schreyer, D. Sulsky et al., “Solving quasi-static equations with the material-point method,” International Journal for Numerical Methods in Engineering, vol. 103, no. 1, pp. 60–78, 2015.

[30] G. H. Kim and I. I. Sohn, “Influence of Li2O on viscous behaviour of CaO-Al2O3-12 mass% Na2O-12 mass% CaF2 based slags,” ISIJ International, vol. 52, no. 1, pp. 68–73, 2012.

[31] H. Liu, G. Wen, P. Tang, G. Wen, and P. Tang, “Crystallization behaviors of mold fluxes containing Li,” Isij International, vol. 49, no. 6, pp. 843–850, 2009.

[32] Y. Sun, H. Wang, and Z. Zhang, “Understanding the relationship between structure and thermophysical properties of CaO-SiO2-MgO-Al2O3 molten slags,” Metallurgical and Materials Transactions B, vol. 49, pp. 677–687, 2018.
[33] L. Zhirong, Y. Xinchen, and L. Min, "Effect of substituting CaO with BaO and CaO/Al₂O₃ ratio on the viscosity of CaO-BaO-Al₂O₃-CaF₂-Li₂O Mold flux system," *Metallurgical and Materials Transactions B*, vol. 9, no. 2, pp. 1–11, 2019.

[34] K. C. Mills, “The influence of structure on the physico-chemical properties of slags,” *ISIJ International*, vol. 33, pp. 148–155, 1993.