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Congregated electron phase and Wagner model applied in titanium distribution behavior in low-titanium slag

Zhen-yang WANG, Jian-liang ZHANG, Xiang-dong XING, Zheng-jian LIU

School of Metallurgical and Ecological Engineering, University of Science and Technology Beijing,
Beijing 100083, China

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Abstract: For studying the carbon thermal reduction rules of titanium in hot metal and providing a theoretical basis for the blast furnace (BF) hearth protection, the distribution behavior of titanium between low-titanium slag system of $CaO-SiO_2-MgO-Al_2O_3-TiO_2$ and hot metal was studied using analytical reagents in a temperature range from 1350 °C to 1600 °C. Through high temperature melting, rapid quenching, chemical analysis and thermodynamic model calculating, the results showed that the increase of reaction temperature, which improved the titanium distribution $L(Ti)$ and lowered the system activity coefficient γ_{sys}, leads to the rise of equilibrium constant. Combined with Wagner and congregated electron phase models, the data obtained in distribution experiments were used to fit out the Gibbs free energy formula of titanium carbothermic reduction. Finally, the relations between the contents of Si and Ti in hot metal and the titanium load to reach the minimum $w(Ti)$ for the formation of TiC were given.

Key words: titanium; distribution behavior; activity coefficient model; hearth protection; titanium load

1 Introduction

The premature erosion of hearth refractories in blast furnace (BF) has become one of the main factors limiting the campaign life [1]. At present, measures to extend the hearth life include intensifying hearth wall cooling, plugging tuyeres, decreasing production, and adding titanium-rich materials [2,3]. The so-called “titanium bear”, which is a precipitate of carbide, nitride and carbonitride of titanium, may form in the BF hearth area if TiO_2 presents in the feed [4]. It can minimize the hearth wall erosion and extend the BF campaign life.

Recently, the researches have mainly focused on the characteristics of high titanium slag ($w(TiO_2)$>10%) when vanadium-bearing titanomagnetite as a main ore is charged into BF [5]. The low-titanium slag ($w(TiO_2)$<5%), which is formed in the condition of titanium ball or iron sand as a protection hearth agent presented slightly in the BF feed, was less studied. LI et al [6] pointed out that the effective titanium charging content for carbonitride formation is 3.6−5.2 kg/t. HE et al [7] studied the phase transition process of TiO_2 carbothermal reduction, which is $TiO_2 \rightarrow Ti_nO_{2n-1}(n\geq4) \rightarrow Ti_3O_5 \rightarrow Ti(N,O) \rightarrow Ti(C,N,O) \rightarrow Ti(C,N)$. However, the research related to carbothermal reduction behavior of low titanium slag using the thermodynamic model mentioned below was limited.

Through simulating the composition of low titanium slag and hot metal, the distribution behavior of Ti under the condition of low-titanium slag was studied using the model of WAGNER [8] and congregated electron phase. A series of thermodynamics parameters and formulas were received, which provided a theoretical basis for the BF hearth protection.

2 Experimental

2.1 Experimental materials

The materials used in the experiment were analytical reagent grade powders. The species and purities are shown in Table 1.

The experimental reagents of CaO, SiO_2, Al_2O_3, MgO, and TiO_2 were roasted at 1000 °C in argon atmosphere for 2 h. The carbonate and hydroxide in the reagents were decomposed during the heating, which purified raw materials and reduced experimental error through the removing of CO_2 and H_2O. When roasting

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Corresponding author: Zhen-yang Wang; Tel: +86-10-62332550; E-mail: wangzheny@126.com

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Table 1 Experimental materials and their purity

Material	Component	Purity/%	Supplier
Slag	CaO	98.0	Sinopharm
	SiO_2	99.0	Sinopharm
	Al_2O_3	99.0	Sinopharm
	MgO	98.5	Sinopharm
	TiO_2	98.0	Sinopharm
Metal	Iron powder	98.0	Sinopharm
	Graphite powder	99.0	Sinopharm
Shielding gas	Ar	99.9	AGA Gas

finished, the reagents were cooled down to room temperature for the next premelting experiments.

2.2 Premelting experiment

Slag and iron were mixed up with composition shown in Table 2 and ground in a agate mortar for 40 min to ensure the composition uniformity. Then, the homogeneous slag and iron were respectively put into high purity graphite crucible and heated to 1450 °C for 2 h in argon atmosphere, which can guarantee the adequate slag crystallization and complete iron carburization through. The compositions of premelting samples through chemical analysis are listed in Table 2.

2.3 Carbothermic reduction

Under the present condition of BF in China, the slag quantity is usually about 300 kg/t. Thus, 30 g premelting slag and 100 g carbon-containing iron were put into a high purity graphite crucible as shown in Fig. 1. The crucible, whose dimension was 40 mm in diameter and 100 mm in depth, was fitted with a molybdenum basket and inserted into the constant temperature zone of the tubular resistance furnace. The samples were then heated up to a target temperature at the rate of 5 °C/min and kept for 4 h [9]. The whole heating process was under Ar atmosphere in flow of 3 L/min which can provide protection atmosphere for titanium reduction and prevent the oxidation of molybdenum wire. Finally, the molybdenum basket with samples was taken out from the furnace and quickly quenched into the ice water. The heat treatment pattern is shown in Fig. 2.

3 Results and discussion

3.1 Reaction mechanism and distribution ratio

Carbon and silicon have a great influence on the activity coefficient of titanium in hot metal, so the contents of C and Si in iron were also tested. The compositions of iron and slag after reduction are shown in Table 3.

According to BERGSMA and RICHARD's results [10], the mechanism of Ti carbothermic reduction in hot metal can be described by the following steps: 1) dissolution of TiO_2 in slag phase, 2) reduction of TiO_2, 3) dissolution of Ti into hot metal and emitting of CO out

Table 2 Slag and iron compositions

Condition	Slag composition/%					Basicity	w(C) in iron/%
	CaO	SiO_2	Al_2O_3	MgO	TiO_2		
Before premelting	40.12	34.88	14	8	3	1.15	4.5
After premelting	40.45	35.91	12.57	7.99	3.08	1.13	4.9

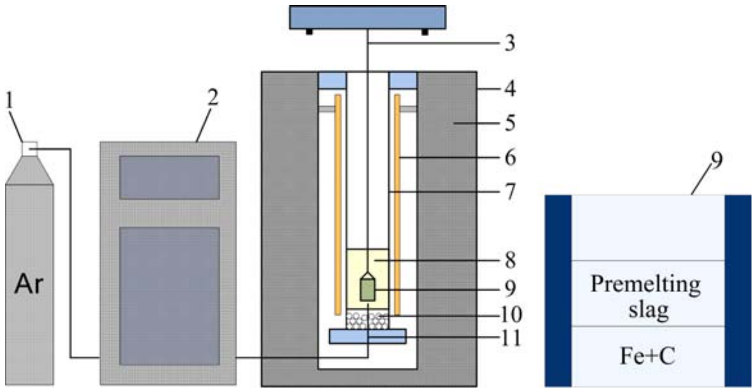

Fig. 1 Tubular resistance furnace and crucible diagram: 1—Shielding gas; 2—Process control system; 3—Molybdenum basket; 4—Tubular resistance furnace; 5—Fire resistant cotton; 6—Silicon-molybdenum rods; 7—Alundum tube; 8—Constant temperature zone; 9—Graphite crucible; 10—Alundum balls; 11—Platinum rhodium thermocouple

of slag, and 4) formation of solid particle TiC because of solubility. The reaction mechanism can be shown as Fig. 3.

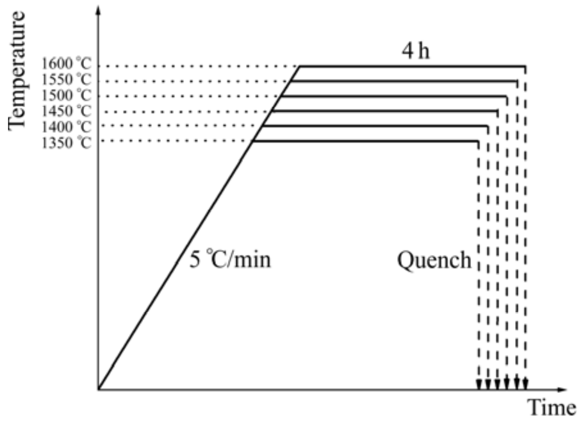

Fig. 2 Experimental heat treatment pattern

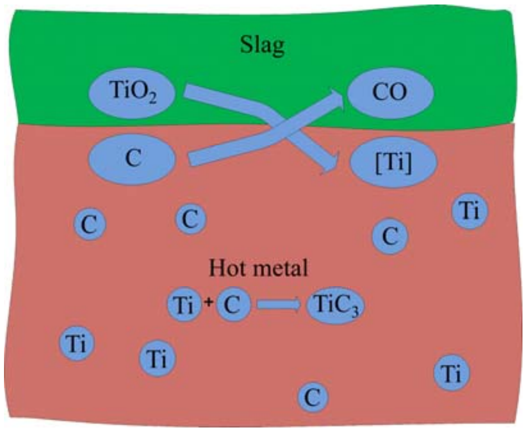

Fig. 3 Model of titanium reaction between liquid slag and hot metal

The main reactions of titanium between iron and slag are as follows:

$TiO_2+2[C]=[Ti]+2CO$

$$K(\mathrm{Ti})=\frac{w(\mathrm{Ti})\gamma(\mathrm{Ti})\times(p(\mathrm{CO})/p^{\Theta})^2}{x(\mathrm{TiO_2})\gamma(\mathrm{TiO_2})\times(a(\mathrm{C}))^2} \tag{1}$$

$[Ti]+[C]=TiC(s)$

$$K(\mathrm{TiC})=\frac{a(\mathrm{TiC})}{w(\mathrm{Ti})\gamma(\mathrm{Ti})\times a(\mathrm{C})} \tag{2}$$

where K(Ti) and K(TiC) represent equilibrium constants of Reaction (1) and (2), w(Ti) and $x(TiO_2)$ are the mass fraction of Ti in metal phase and mole fraction of TiO_2 in slag phase respectively, γ(Ti) and $\gamma(TiO_2)$ indicate the activity coefficients of Ti and TiO_2, respectively. The equilibrium partial pressure of carbon monoxide is given by p(CO).

According to Raoult's law, taking the purity as a standard, the activities of carbon approximates to 1 if carbon is at a saturated state dissolved in hot metal. While the other components use 1% solution as standard state. Since the reaction happened in an open system, the $p(\mathrm{CO})/p^{\Theta}$ can be considered as 1. As the form of pure solid particles existing in hot metal, the activity of titanium carbide a(TiC) is equal to 1 [11,12]. Thus, Eqs. (1) and (2) can be simplified as

$$K(\mathrm{Ti})=\frac{w(\mathrm{Ti})}{x(\mathrm{TiO_2})}\times\frac{\gamma(Ti)}{\gamma(\mathrm{TiO_2})} \tag{3}$$

$$K(\mathrm{TiC})=\frac{1}{w(\mathrm{Ti})\gamma(\mathrm{Ti})} \tag{4}$$

In Eq. (3), the group containing the content of titanium in hot metal and slag can be termed as the "distribution ratio," L(Ti), and the activity coefficients group can be defined as the "system activity coefficient", γ_{sys}, which are given as

$$L(\mathrm{Ti})=\frac{w(\mathrm{Ti})}{x(\mathrm{TiO_2})} \tag{5}$$

$$\gamma_{\mathrm{sys}}=\gamma(\mathrm{TiO_2})/\gamma(\mathrm{Ti}) \tag{6}$$

Thus, Eq. (3) can be written to express the equilibrium constant as a function of distribution ratio and system activity coefficient:

$$K(\mathrm{Ti})=L(\mathrm{Ti})/\gamma_{\mathrm{sys}} \tag{7}$$

The equilibrium constant K(Ti) will remain the same under certain conditions of temperature and pressure. Thus, the titanium distribution ratio L(Ti)

Table 3 Slag and iron compositions after reduction

Temperature/°C	Slag composition/%					Iron composition/%		
	CaO	SiO_2	Al_2O_3	MgO	TiO_2	C	Si	Ti
1350	41.38	34.64	13.07	8.29	2.62	4.51	0.15	0.052
1400	42.35	33.42	13.36	8.36	2.51	4.39	0.34	0.065
1450	43.05	32.58	13.53	8.45	2.39	4.24	0.47	0.083
1500	43.64	31.62	13.61	8.79	2.34	3.92	0.62	0.109
1550	44.26	31.11	13.66	8.82	2.15	3.71	0.70	0.136
1600	44.49	30.53	13.74	9.17	2.07	3.56	0.79	0.172

between slag and hot metal is only related to the system activity coefficient γ_{sys} when temperature and pressure keep unchanged. The reduction degree of titanium from slag phase migrating to hot metal can be expressed as L(Ti). While the γ_{sys}, which is the activity coefficients ratio of reactants and products, represents the titanium reduction potential between liquid slag and hot metal. As shown in Eq. (7), L(Ti) and γ_{sys} are positive correlation.

In titanium balanced system of liquid slag and hot metal, when a parameter, such as a component content, has changed, it will cause a variation of titanium reduction potential, which leads to a change of L(Ti) between liquid slag and hot metal. This process can be quantificationally described as Eqs. (5)−(7). That is, the changed conditions of titanium balanced system will influence the activity coefficient of titanium in the liquid slag and hot metal phase and finally the system activity coefficient γ_{sys}. As a result, the titanium distribution ratio, L_{Ti}, will change.

The TiO_2 mass fraction in Table 3 can be converted to mole fraction through Eq. (8). Combined the data in Table 3 with Eq. (5), the relationship between distribution ratio L(Ti) and temperature is obtained, as shown in Fig. 4.

$$x(\text{TiO}_2)=\frac{w(\text{TiO}_2)}{M(\text{TiO}_2)\sum\frac{x(i)}{M(i)}} \tag{8}$$

where i means slag components of CaO, SiO_2, MgO, Al_2O_3, TiO_2 and $M(i)$ is the relative molecular mass of component i.

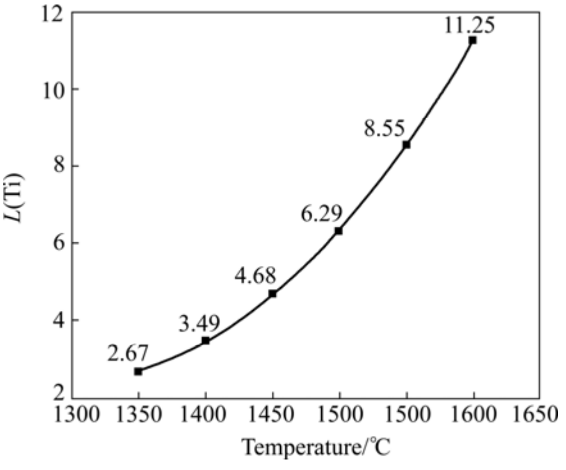

Fig. 4 Titanium distribution L(Ti) along with change of temperature

Indicates that the titanium distribution ratio increases with carbothermic reduction temperature increasing. L(Ti) will be enhanced from 2.67 at 1350 °C up to 11.25 at 1600 °C. The increase of reaction temperature can result in a significant increase in titanium recovery, which is beneficial to improving the content of Ti in hot metal.

3.2 Activity coefficient of titanium in metal and slag phase

Wagner model can be used to obtain activity coefficient of titanium in multicomponent metal phase. The activity interaction coefficients of titanium in hot metal at a certain temperature range from 1350 °C to 1600 °C are shown in Table 4 [13]. The activity coefficient of titanium under a specific composition can be received from Eq. (9).

$$\lg\gamma(\text{Ti})=\sum e_{\text{Ti}}^{j}w(j) \tag{9}$$

where j represents the elements of C, Si and Ti in hot metal.

Table 4 Activity interaction coefficients e_{Ti}^{j} of elements in hot metal at different temperatures

Temperature/°C	C	Si	Ti
1600	−0.165	0.050	0.013
1550	−0.171	0.052	0.013
1500	−0.178	0.054	0.014
1450	−0.184	0.056	0.015
1400	−0.192	0.058	0.015
1350	−0.199	0.060	0.016

The activity coefficients of TiO_2 in slag phase can be obtained by the model of congregated electron phase [14], which are expressed as Eqs. (10) to (13). The atomic energy scalar χ will be used in the calculation process, as seen in Table 5 [13].

$$\varepsilon_{\text{Ti}j}=\frac{1}{2}(\chi_{\text{Ti}}^{1/2}-\chi_{j}^{1/2})^{2} \tag{10}$$

$$\psi_{(\text{Ti})}^{-1}=\sum x(j)\exp[-\varepsilon_{\text{Ti}j}/(RT)] \tag{11}$$

$$a(\text{TiO}_2)=x(\text{TiO}_2)\times\gamma(\text{TiO}_2)=x(\text{Ti})\times\psi(\text{Ti}) \tag{12}$$

$$\gamma(\text{TiO}_2)=\frac{x(\text{Ti})\times\psi(\text{Ti})}{x(\text{TiO}_2)} \tag{13}$$

where ε represents the exchanging position energy of adjacent atom. ψ(Ti) and x(Ti) respectively mean activity coefficient and mole fraction of titanium atom in slag.

Table 5 Atomic energy scalar used in calculation process

Element	χ/(kJ·mol^{-1})
Ca	104.60
Si	171.54
Al	125.52
Mg	146.44
Ti	133.89
O	1255.20

The activity coefficient of Ti in hot metal γ(Ti), the activity coefficient of TiO_2 in slag phase $\gamma(TiO_2)$ and the system activity coefficient γ_{sys} at different reaction temperature are shown in Fig. 5.

As seen in Fig. 5, when the reaction temperature goes up from 1350 °C to 1600 °C, γ(Ti) increases gradually, from 0.184 to 0.220, while $\gamma(TiO_2)$ shows a trend of decrease, from 0.983 down to 0.971. Since the system activity coefficients γ_{sys} are correlated with $\gamma(TiO_2)$ positively and γ(Ti) negatively, γ_{sys} declines from 5.352 to 4.422. It is apparent that the titanium reduction potential between liquid slag and hot metal decreases with the temperature going up. However, the distribution ratio of titanium rises instead. These opposite variation trends of γ_{sys} and L(Ti) indicate that the equilibrium constant of titanium reduction increases following the temperature. Combined L(Ti) with γ_{sys}, a series of thermodynamic parameters and formulas can be received.

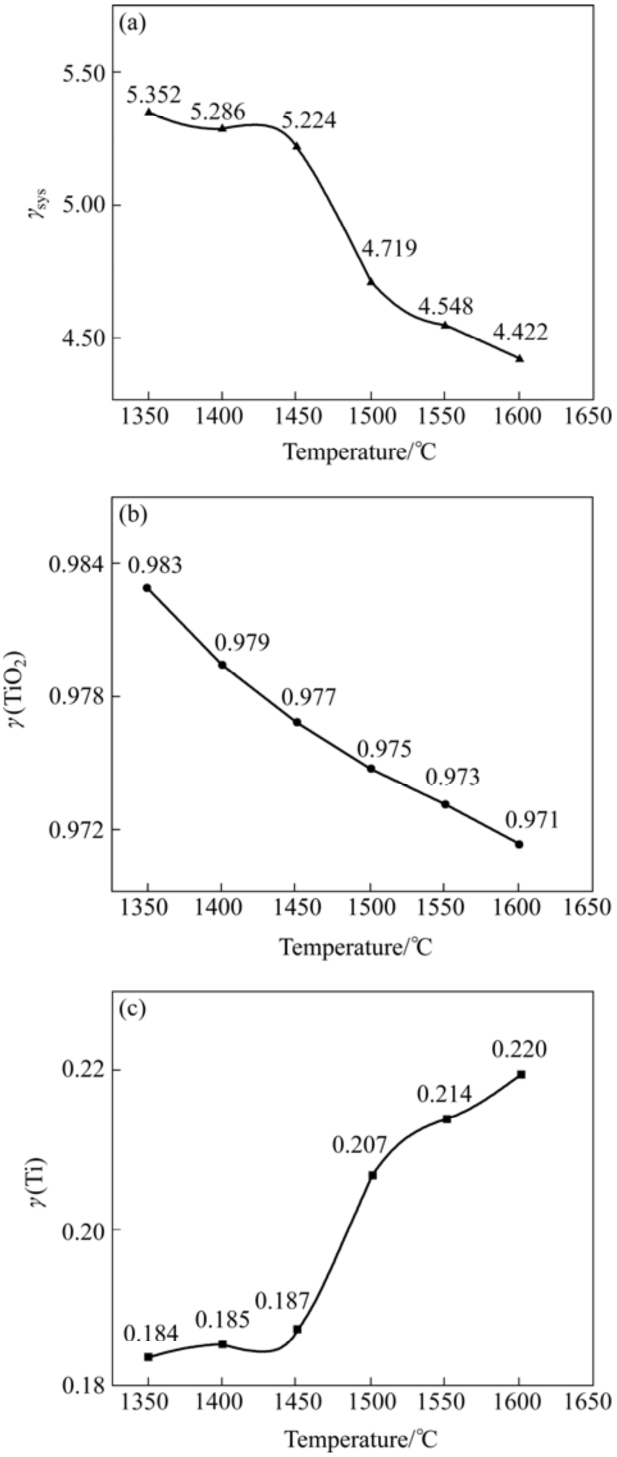

Fig. 5 Change of activity coefficient with temperature

3.3 Thermodynamics calculation of titanium carbothermic reduction

The standard Gibbs free energy change for Reactions (14) and (15) can be calculated from the data of WANG [15] and LI et al [6], which were applicable over the temperature range from 1300 °C to 1700 °C, as seen in Eqs. (14) and (15).

$$TiO_2+2[C]=[Ti]+2CO$$

$$\Delta G^{\Theta}_{Ti}/(J\cdot mol^{-1})=164060-95.05T \tag{14}$$

$$[Ti]+[C]=TiC_s$$

$$\Delta G^{\Theta}_{TiC}/(J\cdot mol^{-1})=-153700+57.53T \tag{15}$$

Based on the system activity coefficients and distribution ratios of titanium obtained above, the equilibrium constant K and Gibbs free energy curve can be received using Eqs. (4), (7) and Eqs. (14), (15). The data from experiments of WANG [15] and LI et al [6] are demonstrated in Fig. 6.

From Fig. 6(a), with the increase of reaction temperature, the equilibrium constant K(Ti) goes up gradually, which promotes the course of titanium carbothermal reduction reaction. The K(Ti) of present study is slightly larger than the data from WANG [15]. It can come down to the product of TiC in the hot metal, which accelerates the reduction reaction. K(Ti) of the present study is a little higher. The equilibrium constant K(TiC) based on both of the present study and LI [6] are plotted against the reaction temperature in Fig. 6(c). It shows that K(TiC) decreases obviously when the temperature varies from 1350 °C to 1600 °C. This tendency also verifies the formation of TiC in the hearth refractory breakage because of cooling. From Figs. 6(b) and (d), the Gibbs free energy change formulas of titanium carbothermal reduction based on experiments are fitted, which are $\Delta G^{\Theta}_{Ti}/(J\cdot mol^{-1})=169251-97.93T$ and $\Delta G^{\Theta}_{TiC}/(J\cdot mol^{-1})=-143370+49.18T$.

3.4 Volume of titanium-bearing feed to protect BF hearth refractory

The content of silicon is a common evaluation standard to hot metal. Since the reduction of silicon is closely associated with hearth temperature, silicon is

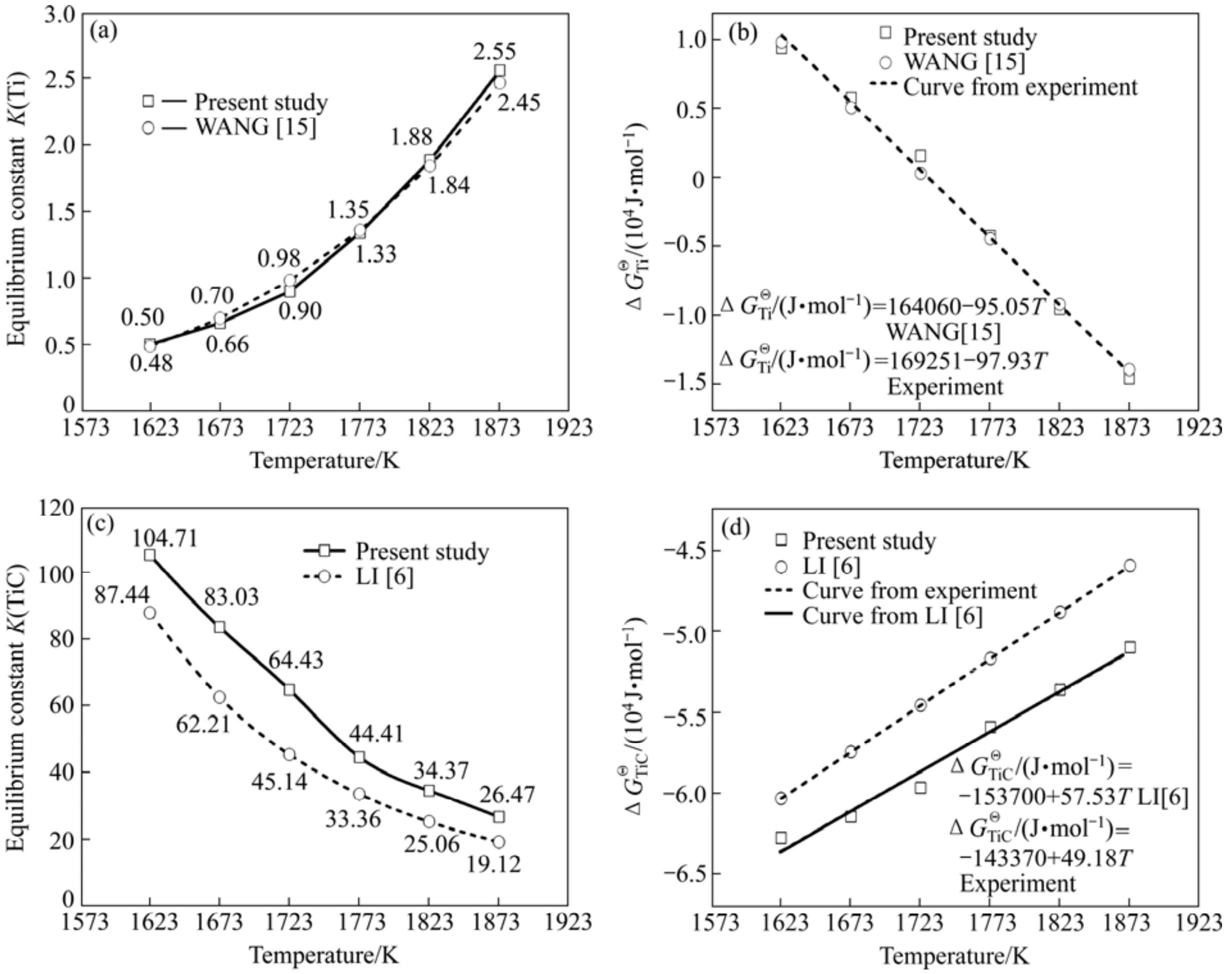

Fig. 6 Equilibrium constant K and ΔG^{Θ} of titanium reduction along with temperature: (a), (b) K(Ti), $\Delta G_{\text{Ti}}^{\Theta}$ of Reaction (1) based on present study and WANG [15]; (c), (d) K(TIC), $\Delta G_{\text{Ti}}^{\Theta}$ of Reaction (2) based on present study and LI [6]

commonly used to represent the chemical heat of hot metal. To obtain a more utility parameter for actual production, the relationship between distribution ratio of titanium and silicon is fitted based on the experimental data obtained above, as shown in Eq. (16) and Fig. 7.

$$\frac{w(\text{Ti})}{w(\text{TiO}_2)}=142.884\left(\frac{w(\text{Si})}{w(\text{SiO}_2)}\right)^2-1.496\frac{w(\text{Si})}{w(\text{SiO}_2)}+0.0247 \tag{16}$$

Since high hearth temperature is beneficial to the reduction of silicon, the distribution ratios of silicon and titanium have the positive correlation. Taking 35% as a typical content of SiO_2 in slag and 5−20 kg/t as a TiO_2 load into BF, the content of titanium in hot metal as a function of silicon and TiO_2 load can be plotted using Eq. (16), as shown in Fig. 8. Thus, w(Ti) can be estimated directly based on the quantity of effective charging TiO_2 and w(Si).

ZHANG [16] showed that when the content of titanium in hot metal reached 0.1%−0.18%, it can effectively protect the BF hearth refractories and keep a smooth operation at same time. Based on the titanium distribution ratio obtained above, the minimum titanium load for a typical BF slag amount of 300 kg/t is shown in Fig. 9.

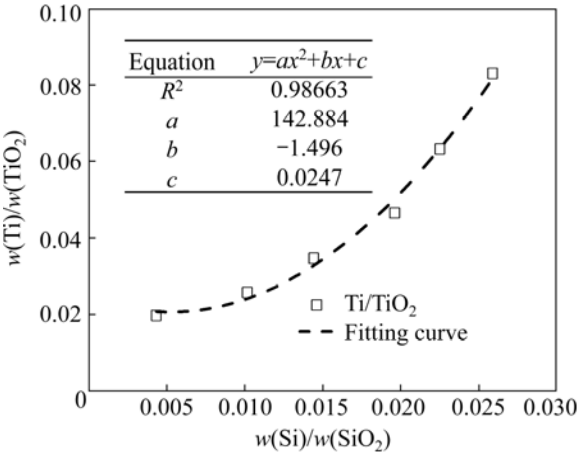

Fig. 7 Relationship of mass distribution ratio between titanium and silicon

From Fig. 9, since L(Ti) and reduction potential increase with the hearth temperature going up, the

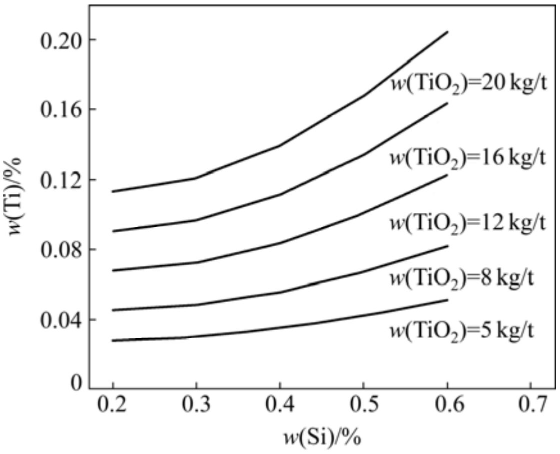

Fig. 8 Content of titanium in hot metal as function of silicon and TiO_2 load

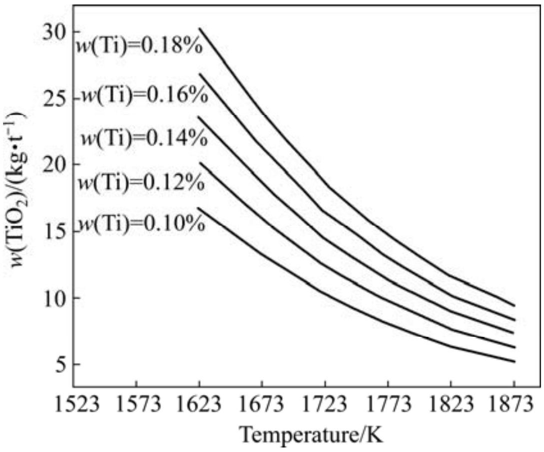

Fig. 9 Predicted minimum titanium load required for protection of hearth in BF

volume of TiO_2 load required for protecting refractories decreases gradually. For a representative hearth temperature of 1773 K, the load of TiO_2 in BF feed is in the range of 8.11−14.59 kg/t, which indicates that the prediction according to experiment data agree well with that used in BF practical operation.

4 Conclusions

1) Through defining the distribution ratio of titanium L(Ti) and system activity coefficient γ_{sys}, the equilibrium constant of titanium carbothermal reduction reaction K(Ti) can be expressed as the ratio of L(Ti) and γ_{sys}. System activity coefficient γ_{sys} can be used to represent Ti reduction potential.

2) Activity coefficient of titanium in metal phase goes up gradually along with the increase of reduction temperature, while the activity coefficient of titanium dioxide in slag phase shows a trend of decrease, which leads to the decrease of system activity coefficient. Since L(Ti) is correlated with temperature positively, the K(Ti) increases with the rise of temperature. K(Ti) of the present study is a little higher than the published, which can come down to the appearance of TiC.

3) Based on the model of Wagner and congregated electron phase, the Gibbs free energy change formulas of titanium carbothermal reduction are fitted, which are $\Delta G^{\Theta}_{\mathrm{Ti}}$ /(J·mol^{-1})=169251−97.93T and $\Delta G^{\Theta}_{\mathrm{TiC}}$ /(J·mol^{-1})= −143370+49.18T.

4) Through the fitted formula between silicon and titanium distribution ratio, the relation of w(Si) and w(Ti) is received at different titanium loads, which is beneficial to making a quick judgment in practical operation. Finally, the predicted titanium load to reach the minimum w(Ti) for BF hearth protection is given.

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凝聚电子相与 Wagner 模型在低钛渣下钛的分配行为中的应用

王振阳，张建良，邢相栋，刘征建

北京科技大学 冶金与生态工程学院 北京 100083

摘　要：为研究铁水中钛元素碳热还原反应规律，提供高炉护炉理论依据，利用高温熔炼、急速淬火、化学分析以及热力学模型计算等方法，在实验室条件下利用分析纯试剂研究在 1350~1600 °C 间钛在低钛渣系 $CaO-SiO_2-MgO-Al_2O_3-TiO_2$ 与铁水间的分配行为。研究结果表明，随着反应温度的增加，钛的分配比 L(Ti)增加，但系统活度系数 γ_{sys} 降低，从而导致反应平衡常数升高。结合 Wagner 与凝聚电子相模型，通过对实验数据进行拟合，得到钛碳热还原反应的吉布斯自由能公式。最后，结合实验所得结果，给出了高炉铁水中 w(Si)与 w(Ti)含量的关系以及可以达到护炉效果的最小入炉钛负荷。

关键词：钛；分配行为；活度系数模型；护炉；钛负荷

(Edited by Yun-bin HE)