J. Min. Metall. Sect. B-Metall., 56 (2) (2020) 153 - 160

Journal of Mining and Metallurgy, Section B: Metallurgy

EXPERIMENTAL DETERMINATION OF ACTIVITY INTERACTION COEFFICIENTS OF COMPONENTS IN Si-B-Fe AND Si-B-Al TERNARY SYSTEMS AT 1723 K

F. Yang [a, b], Y.-Q. Zhou [b], J.-J. Wu [a, b*], W.-H. Ma [a, b*], Y. Lei [a, b]

[a*] Key Laboratory for Nonferrous Vacuum Metallurgy of Yunnan Province, Kunming University of Science and Technology, People's Republic of China

[b] Faculty of Metallurgical and Energy Engineering, Kunming University of Science and Technology, People's Republic of China

(Received 31 July 2019; accepted 14 February 2020)

Abstract

The interactions among impurity components in Si-based solution are the important thermodynamic parameters for the purification of silicon materials. A "same concentration" method was used to determine the activity interaction coefficients of Fe to B and Al to B in the silicon solution. Fe and Al were respectively dissolved into the binary Si-B solution at 1723 K with the holding time of 5 h, 7 h, 9 h, and 11 h. The equilibrium concentrations of Fe, B in the Si-B-Fe system and Al, B in the Si-B-Al system were determined. The interaction coefficients of Fe to B and Al to B were obtained by fitting the solubility data of B, Fe, and Al. The solubility relationships between B and [%Fe], and between B and [%Al] were obtained, respectively. It was found by the SEM and EPMA pictures of the samples that the third component Fe or Al added to the binary Si-B solution was alloyed, which verifies the accuracy of the experimental determination results. The significance of the activity interaction coefficient of B on boron removal from industrial silicon was analyzed.

Keywords: *Si-based solution; Ternary system; Activity interaction Coefficient; Saturation solubility; Physical characterization*

1. Introduction

Solar grade silicon (SoG-Si) is a key material for solar photovoltaic conversion. A metallurgical route for producing SoG-Si that employs relatively inexpensive metallurgical grade silicon (MG-Si, ~99%) as the raw material is believed to be a promising approach for fabricating solar cells [1-3]. However, various impurities in silicon such as iron, aluminum, boron, etc., have a great negative impact on the photoelectric conversion performance of solar grade silicon [4]. In the process of metallurgical production of industrial silicon, boron is mainly removed by refining outside the furnace [5]. The temperature of silicon refining is around 1723 K so the thermodynamic parameters ε_B^{Fe} and ε_B^{Al} about the phase equilibria and the liquid phase are necessary, since the boron removal from silicon by refining is relevant to the thermodynamic parameters such as solubility and activity in silicon [6-8]. Currently, there are no details on the thermodynamic parameters about boron removal from silicon under high temperature conditions.

Therefore, the research on the thermodynamic properties of metallurgical grade silicon has always been a research hotspot in the silicon industry [9]. Liu [10] et al. used the MIVM model to investigate the thermodynamic behavior of Al and Fe in Si solution in the vacuum environment, and calculated the activity interaction coefficients between Fe and Al. Tao [11-13] used the MIVM model to calculate the interaction coefficient of each component in the Si-Fe-Al system, and obtained the activity interaction coefficient of Fe to Fe, Fe to Al, and Al to Al in the silicon solution at 1687 K. The iso activity curves of the Fe and Al components in the liquid Si-Al-Fe ternary system at 1823 K are drawn. Cui et al. [14] conducted the thermodynamic optimization of the binary Ca-Fe and the ternary Ca-Fe-Si systems based on the critical evaluation of all phase diagrams and thermodynamic properties data available in the literature, and predicted several pseudo-binary sections and isopleths in the ternary Ca-Fe-Si system. Iwata et al. [15] predicted the activity coefficients and the interaction coefficients of Ti, Fe, Al, and Pb elements in the infinite dilute Si solutions by using first-

**Corresponding author: dragon_wu213@126.com; mwhsilicon@126.com*

https://doi.org/10.2298/JMMB190731006Y

principles calculations based on density functional theory. They compared the theoretical calculations with the reported experimental results and found that considering the excess entropy would reduce the difference between theoretical and experimental measurements. Yang et al. [16] used the atom and molecule co-existence theory to calculate the thermodynamic properties of Si-Fe-Ca system, and obtained the activity interaction coefficient of Ca to Fe (ε_{Fe}^{Ca}) in Si solution at 1723-1873 K. Noguchi et al [17] determined the activity coefficient of B and the activity interaction coefficient of B and N in Si by equilibrating solid BN and liquid Si in a nitrogen atmosphere from 1723 to 1923 K, and obtained the favorable conditions for removing boron in Si liquid. Applying the atom and molecule co-existence theory model to the Si-Fe binary system, Yang et al. [18] studied the infinite dilute activity coefficient and the self-interaction coefficient of Fe in the temperature range of 1693-1993 K. Zhou et al. [19] used the "same activity" method to determine the activity interaction coefficient of Al to Fe in Si solution at 1663-1723 K. Miki et al. [20-22] used the chemical equilibration method and the Knudsen effusion method to determine the thermodynamic properties of elements such as Al, Ca, Mg, Ti, and Fe in Si, and obtained the relationship between the infinite activity coefficients of Al, Ca, and Mg in Si liquid and temperature. In addition, they also obtained the relationship between the activity interaction coefficient and the temperature of each element in Si alloys.

We determined the interaction coefficients ε_B^{Fe} in the Si-B-Fe and ε_B^{Al} in the Si-B-Al systems using the "same concentration" method at 1723 K. In order to ensure the dissolution balance of the B, Fe, and Al components at 1723 K, the alloying samples were kept at the temperature for the 5 h, 7 h, 9 h and 11 h, respectively, in the process of experimental. The relationship between the saturated solubility of B, and [%Fe] or [%Al] were obtained. At the same time, the microstructures of the Si-B-Fe and Si-B-Al alloying samples were physically characterized to verify the accuracy of the experimental results.

2. Experimental

The Fe (>99.97%), Al (>99.95%), Si (>99.99%), and B (>99.9%) powders were used as the raw materials in the experiments. As shown in the Si-B binary phase diagram (Fig. 1) [23], the boron concentration on the liquidus at 1723 K is about 5.5% mass ratio. Therefore, the raw materials were matched according the liquidus at 1723 K and the raw material composition used for preparing the experimental alloys is shown in Table 1. An excess of B in Si-B-Fe and Si-B-Al systems was ensured.

The high-purity Si, B, Fe or Al were weighed and mixed uniformly and then placed in a corundum crucible of φ20-mm*33-mm, which was encased in a graphite crucible of φ63-mm*90-mm. Since the content of Fe and Al added in the experiment is high, the influence of Al in corundum crucible on the experiment can be neglected. The crucibles were then placed in a vacuum tubular resistance furnace as shown in Fig. 2. In order to ensure that the materials were not oxidized, the furnace tube was first evacuated, and then a high purity argon gas (99.99%) was continuously supplied during the experiment. The temperature was raised to 1723 K and kept for 5, 7, 9, and 11 hours, respectively. After the full dissolution of

Table 1. *Batching schemes of dissolution equilibrium experiments for Si-B-Fe and Si-B-Al systems at 1723 K*

Exp.	Al/Fe (g)	B (g)	Si (g)
1	0	0.57	9.43
2	1	0.6	9.43
3	2	0.7	9.43
4	4	0.8	9.43

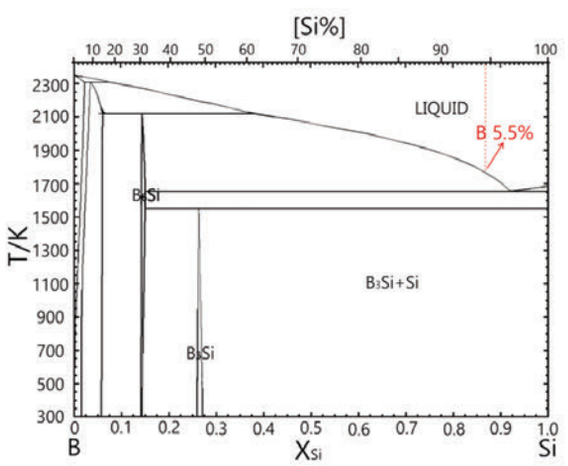

Figure 1. *Si-B binary phase diagram*

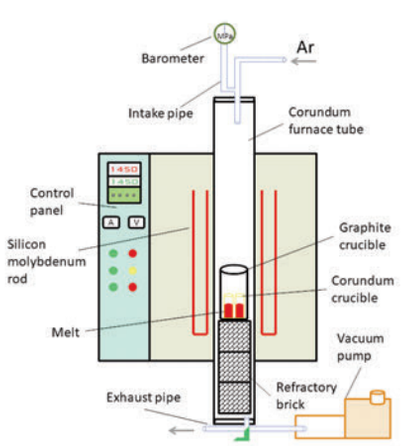

Figure 2. *Vacuum/atmosphere tubular resistance furnace and its structure*

B and Fe or Al in the silicon solution, the high-temperature graphite crucible was quickly extracted from the furnace tube by a molybdenum wire, and the silicon solution was quenched.

The alloying sample was firstly sanded with the sandpaper and then cleaned with alcohol. It was cut into two pieces by a diamond wire cutter. One piece was ground into a powder in an agate mortar (less than 200 mesh) and another was burnished. The contents of B, Fe or Al in the powder samples were measured by the Inductively Coupled Plasma Atomic Emission Spectrometry (ICP-AES, Optima 8000, Perkin Elmer Corporation). The burnished samples were detected by the Scanning Electron Microscopy (SEM, XL30ESEM, Netherlands) and the Electron Probe Microanalysis (EPMA, JXA-8230, Japan Electronics Co., Ltd.). The experimental process is shown in Fig. 3.

3. Results and discussion

3.1 Interaction coefficients ε_B^{Fe} and ε_B^{Al}

The activity interaction coefficient refers to the activity coefficient effect of the component j on another component i in Si-i-j solution, which embodies the correction of the component activity coefficient. In this study, the "same concentration" method was used for the experimental determination work. When the components j and k ... are added to the Si-i binary system, the components in the system reach the concentration balance within a certain time frame, and the effect of the components j and k ... on the activity coefficient of component i can be calculated [24].

In this study, Fe or Al is added to the Si-B binary system, and the effect of Fe or Al on the activity coefficient of B was obtained. The Wagner equations [25, 26] corresponding to the Si-B-Fe system and the Si-B-Al system are shown in the formulas (1) and (2), respectively.

$$\lg f_B = e_B^B[\%B] + e_B^{Fe}[\%Fe] \quad (1)$$

$$\lg f_B = e_B^B[\%B] + e_B^{Fe}[\%Fe] \quad (2)$$

The results of chemical composition analysis by ICP for the Si-B-Fe and Si-B-Al ternary alloy samples at 1723 K with different holding time are shown in Table 2.

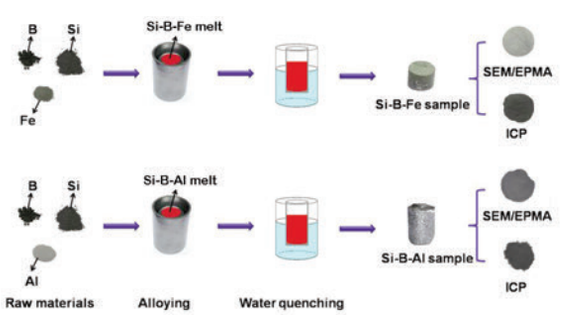

Figure 3. *Experimental flow chart*

Since the boron is at a saturated state, the activity of B in silicon solution is 1.

$$x_B\gamma_B = 1 \quad (3)$$

Given as

$$\gamma_B^0 = \gamma_B / f_B \quad (4)$$

Therefore,

$$f_B = 1/x_B\gamma_B^0 \quad (5)$$

We know from the literature that γ_B^0 is 0.24 [27], so the calculation results of Si-B-Fe and Si-B-Al ternary alloy systems by the formulas (3)-(5) and the data of Table 2 are obtained and shown in Table 3.

According to Table 2 and Table 3, the fitting results of [%Fe] to lgf_B and [%Al] to lgf_B at 1723 K with different holding time in the Si-B-Fe and Si-B-Al ternary alloy systems are shown in Fig. 4(a) and Fig. 4(b). Due to the slight fluctuations in the current and temperature fields of the experimental furnace, there are subtle differences between the samples, but the fitted straight lines of multiple samples can compensate for this difference. It is found from the fitting results that the dissolution equilibrium is reached. The fitting result of 5

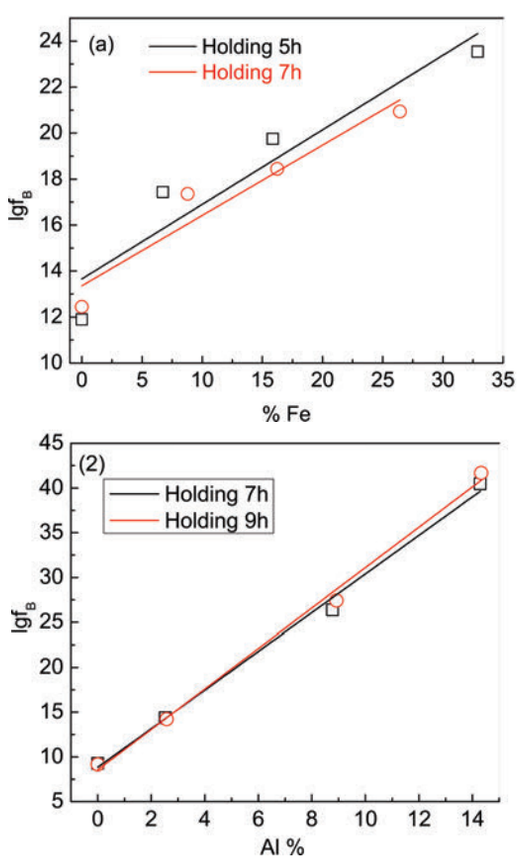

Figure 4. *(a) Fitting results between [%Fe] and* $\lg f_B$ *at 1723 K; (b) Fitting results between [%Al] and* $\lg f_B$ *at 1723 K*

Table 2. *Chemical compositions of components in Si-B-Fe and Si-B-Al systems at 1723 K with different holding time*

Holding time (h)	Si-B-Fe System					Si-B-Al System				
	Sample	1	2	3	4	Sample	1	2	3	4
5	[%B]	4.44	2.98	2.67	2.26	[%B]	2.8	2.62	2.08	1.3
	[%Fe]	0	6.73	15.86	32.89	[%Al]	0	1.28	6.95	13.19
7	[%B]	3.86	2.76	2.61	2.29	[%B]	4.81	3.11	1.69	1.11
	[%Fe]	0	8.79	16.24	26.43	[%Al]	0	2.52	8.77	14.29
9	[%B]	1.95	3.46	3.26	1.16	[%B]	4.79	3.08	1.6	1.05
	[%Fe]	0	9.46	21.74	33.91	[%Al]	0	2.58	8.92	14.33
11	[%B]	2.06	2.48	3.84	1.15	[%B]	4.71	3.21	2.51	1.65
	[%Fe]	0	9.41	21.49	34.18	[%Al]	0	6.96	13.1	17.65

Table 3. *Fitting data of Si-B-Fe and Si-B-Al system at 1723 K*

Holding time (h)	Si-B-Fe system					Si-B-Al system			
	Sample	1	2	3	4	1	2	3	4
5	x_B	0.35	0.239	0.211	0.177	0.318	0.298	0.236	0.148
	lgf_B	11.9	17.43	19.75	23.54	13.1	13.98	17.66	28.15
7	x_B	0.335	0.24	0.226	0.199	0.449	0.29	0.158	0.103
	lgf_B	12.44	17.36	18.44	20.94	9.28	14.37	26.37	40.45
9	x_B	0.2	0.351	0.332	0.117	0.455	0.293	0.152	0.1
	lgf_B	20.83	11.87	12.55	35.61	9.16	14.22	27.41	41.67
11	x_B	0.217	0.26	0.402	0.12	0.391	0.266	0.208	0.136
	lgf_B	19.2	16.03	10.36	34.72	10.66	15.66	20.03	30.64

h holding time is almost consistent with that of 7 h holding time in the Si-B-Fe ternary alloy system, and the fitting result of 7 h holding time is almost consistent with that of 9 h in the Si-B-Al ternary alloy system. Therefore, the concentrations of B and Fe or Al are in a dynamic equilibrium state with the 5 h and 7 h holding time in Si-B-Fe ternary alloy system and the 7 h and 9 h holding time in the Si-B-Al ternary alloy system.

Due to some uncontrollable factors and changes in the Fe and Al contents during the experiment, the saturation solubility of B in the Si solution also changed. However, it can be seen that the content of B is very low relative to the content of Fe and Al, and the solubility change of B is not very significant.Thus, this study ignores the effect of B's own solubility change on the experiment. According to the equations (1) and (2), it is seen that the slope of the fitted straight line is the activity interaction coefficient e_B^{Fe} or e_B^{Al} , which is converted to ε_B^{Fe} or ε_B^{Al} by the formulas (6) and (7).

$$\varepsilon_B^{Fe} = 230\frac{M_{Fe}}{M_{Si}}e_B^{Fe} + \frac{M_{Si} - M_{Fe}}{M_{Si}} \quad (6)$$

$$\varepsilon_B^{Al} = 230\frac{M_{Al}}{M_{Si}}e_B^{Al} + \frac{M_{Si} - M_{Al}}{M_{Si}} \quad (7)$$

The results of ε_B^{Fe} and ε_B^{Al} are shown in Table 4.

Table 4. *Experimental results of activity interaction coefficients at 1723 K*

Parameters	Si-B-Fe system		Si-B-Al system	
	5 h	7 h	7 h	9 h
e_B^{Fe}	0.3243	0.306		
e_B^{Al}			2.1549	2.2541
ε_B^{Fe}	147.31	139.94		
ε_B^{Al}			476.04	497.96

3.2 Physical characterization techniques

The SEM microstructures of the Si-B-Fe and Si-B-Al ternary alloy samples by experiments at 1723 K are shown in Fig. 5. As can be seen, the phases are evenly distributed and there are some black areas in each of the figures. Fig. 6 is the EPMA analysis of each ternary alloy sample. It is found that the black region is the solid solution phase of Si and B, and the white regions in Fig. 6 (b) and (d) are the solid solution phase of Si and Fe. There are Al phase in Fig. 6 (f) and (h). In the alloy samples, the solid solution phases of Fe and

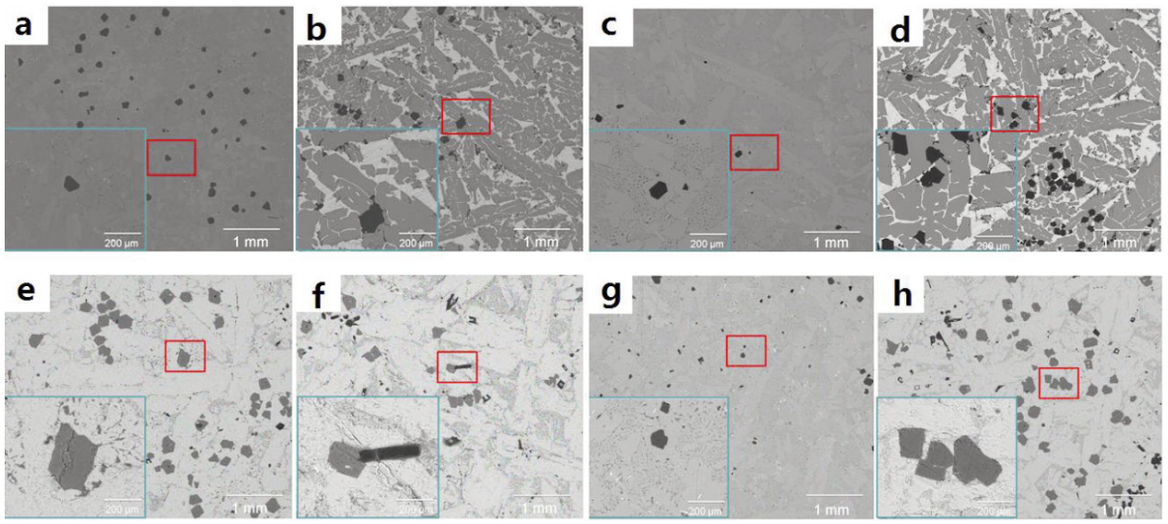

Figure 5. *SEM microstructures of Si-B-Fe and Si-B-Al ternary alloy samples*

B are not found, and almost no solid solution phases of Al and B are found. As can be seen from the Fig. 6 (b) and (d) that B is enriched around the addition Fe, which reduces the B content in the silicon solution. As can be seen from the red circle part of Fig. 6 (f) and (h), most of the aluminum exists alone, and a small amount of aluminum diffuses into the Si-B phase so that the Si-B-Al phase is formed.

From the above analysis, it can be concluded that the affinity between Si, Fe, Al, and B in the Si solution at 1723 K has the relationship of Si-Fe>Si-B>Al-B>Fe-B. Wu et al. [28] used molecular dynamics to simulate the covalent interaction between Si, B, Al, and Fe. That is, in a high temperature solution, Si is more likely to bind to Fe, and B is less inclined to bond with Fe. It was concluded that the covalent interaction strength of Si-Fe is greater than that of Si-B, which is consistent with the experimental results of this study.

3.3 Features of ε_B^{Fe} and ε_B^{Al} on Si purification

The Si-B-Fe and Si-B-Al alloy solutions at 1723 K are in dynamic equilibrium states with 5 h, 7 h, and 9 h holding time, respectively. As shown in Fig. 7(a) and Fig. 7(b), the saturation solubility of boron in the silicon solution decreases with the increase of Fe and Al contents.

Since the affinity of Fe to Si is greater than the affinity of Si and B, Si atoms are more likely to combine with Fe to form a compound, so that the compound formed by Si and B is reduced, resulting in a decrease in the saturation solubility of B. Its atomic behavior diagram is shown in Fig. 8(a). The addition of Al changes the original Si-B phase to the Si-B-Al phase, and Al extrudes a portion of the B atom, reducing the saturation solubility of B in Si. A schematic diagram of its atomic and molecular behavior is shown in Fig. 8(b).

Presently, slag treatment is the most popular method for boron removal from silicon. However, boron removal is disturbed by other impurity components in silicon. The experimental results show that the values of ε_B^{Fe} and ε_B^{Al} are positive and there exists the relationship of $\varepsilon_B^{Al}>\varepsilon_B^{Fe}>0$. The third component Fe or Al will both increase the activity coefficient and decrease the saturation solubility of boron in silicon solution. It is also more beneficial to remove boron from silicon by combining with the slag agent due to the reduction of solubility and the increase of activity coefficient of boron. Therefore, the existence of a small amount of Fe or Al will have a positive effect on boron removal by slag treatment, and the effect of Al is more obvious.

Many researchers have previously studied the activity interaction coefficients of other components to B in Si [26, 29, 30]. The activity interaction coefficients of some elements to B in Si solution at 1723 K are shown in Fig. 9. The interaction coefficients of N, Mg, and Ni to B are positive, and their existence can reduce the content of B in Si. The interaction coefficients of Ca, Ti, and Mn to B are negative, and their existence has an adsorption effect on B. Therefore, the existence of Fe, Al, N, Mg, and Ni in the Si liquid is advantageous for boron removal from industrial silicon and the existence of Ca, Ti, and Mn is unfavorable.

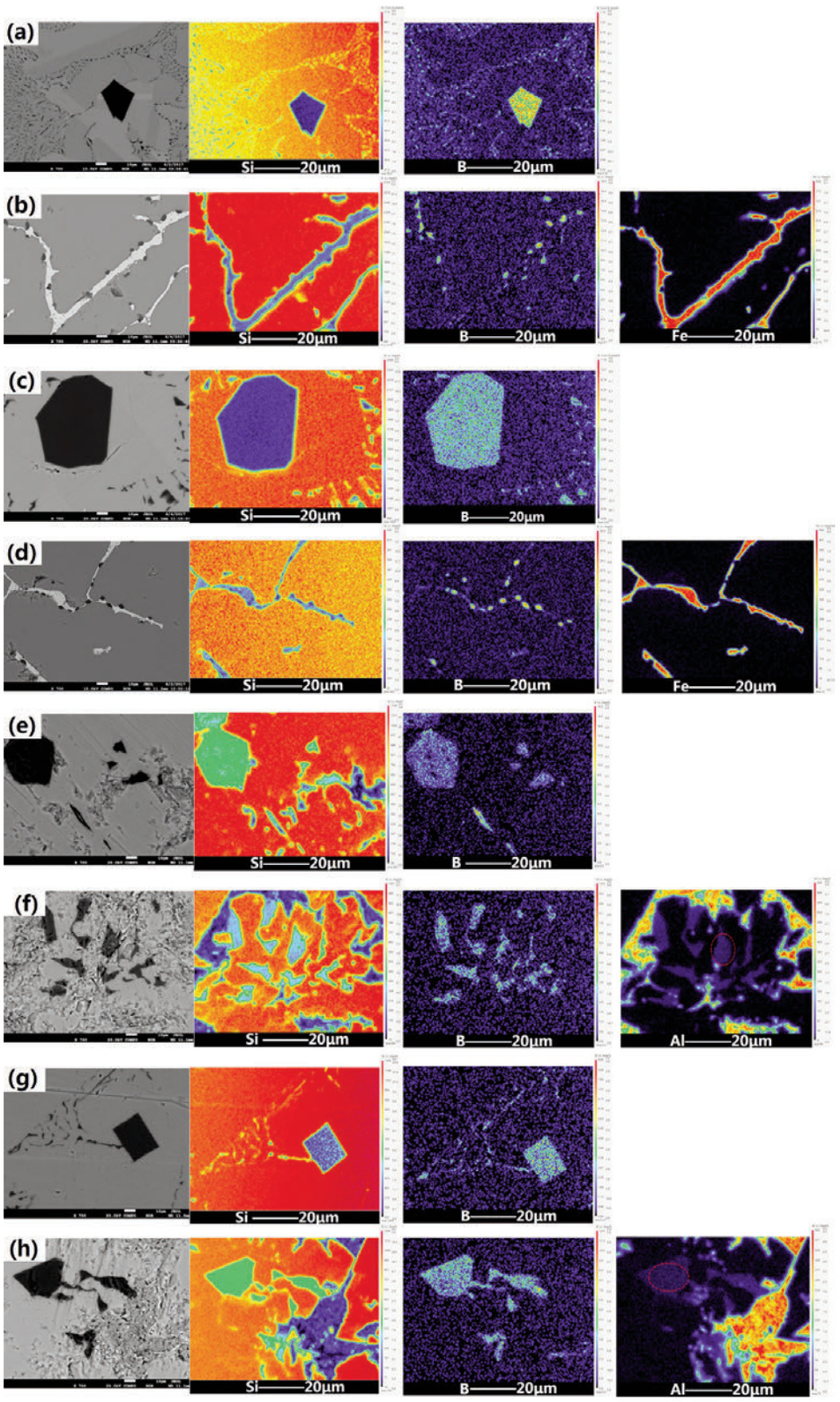

Figure 6. *EPMA analysis of Si-B-Fe and Si-B-Al ternary alloy samples: (a) Si-B-Fe sample 1 for 5 h; (b) Si-B-Fe sample 3 for 5 h; (c) Si-B-Fe sample 1 for 7 h; (d) Si-B-Fe sample 3 for 7 h; (e) Si-B-Al sample 1 for 7 h; (f) Si-B-Al sample 3 for 7 h; (g) Si-B-Al sample 1 for 9 h; (h) Si-B-Al sample 3 for 9 h*

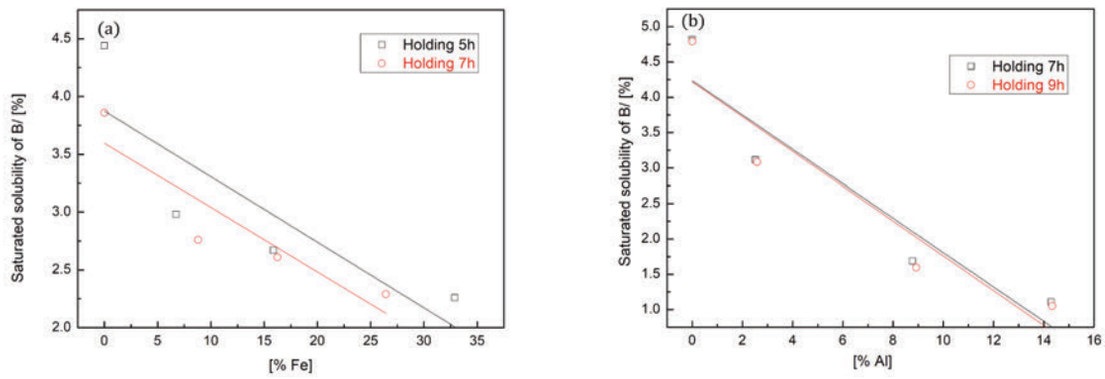

Figure 7. *(a) Change of saturated solubility of B in silicon solution with the content of Fe; (b) Change of saturated solubility of B in silicon solution with the content of Al*

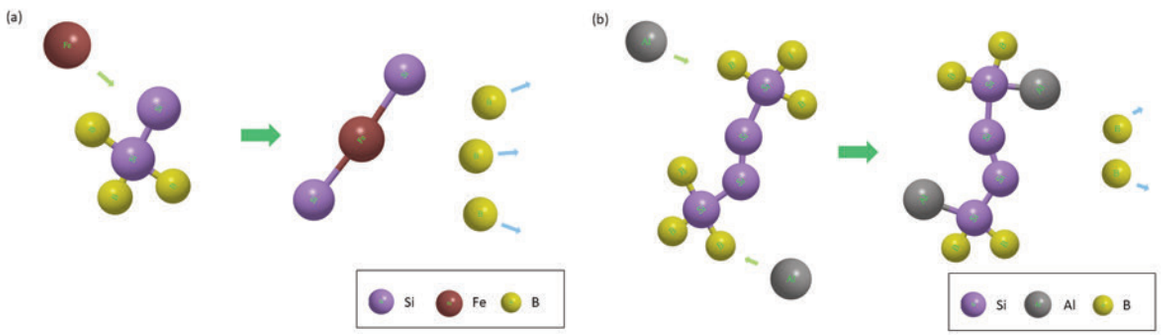

Figure 8. *(a) Schematic diagram of substitution of Fe atom for B atom; (b) Schematic diagram of Al atom replacing B atom*

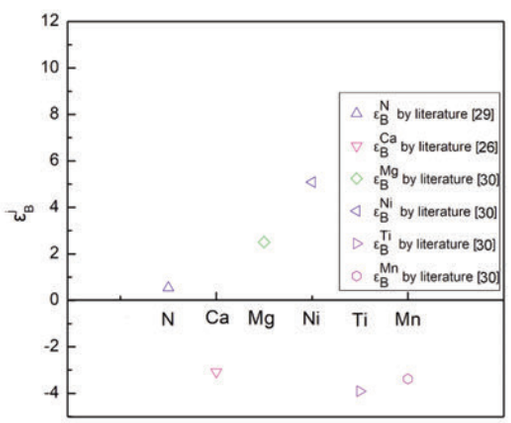

Figure 9. *Activity interaction coefficient of each component to B in Si solution at 1723K [26, 29, 30]*

4. Conclusions

Using the "same concentration" method, the activity interaction coefficients of Fe to B and Al to B in Si-B-Fe and Si-B-Al ternary systems and other conclusions were determined by solubility equilibrium experiments at 1723 K.

(1) The interaction coefficients ε_B^{Fe} and ε_B^{Al} at 1723 K are 2.7076 and 9.8287, respectively. The saturated solubility of B in Si-B-Fe and Si-B-Al ternary alloy systems at 1723 K decreases gradually with the increase of [%Fe] and [%Al].

(2) The microstructures of Si-B-Fe and Si-B-Al ternary alloy samples were characterized using SEM and EPMA techniques to testify the uniformity of alloy samples dissolved at 1723 K. Affinity relationship between Si, Fe, Al, and B was found: Si-Fe> Si-B> Al-B> Fe-B, which verifies the accuracy of the results.

(3) The significance of ε_B^{Fe} and ε_B^{Al} is analyzed from the industrial point of view. The existence of a small amount of Fe and Al is benefit for Si slag refining removes B.

Acknowledgements

The authors wish to acknowledge the financial support on this research from National Natural Science Foundation of China (51574133 and U1902219), the major R&D project of Yunnan in China (2019ZE00701) and the Program for Innovative Research Team in University of Ministry of Education of China (IRT_17R48)

References

[1] K. Morita, T. Miki, Intermetallics, 11 (11) (2003) 1111-1117.

[2] M. Li, T. Utigard, M. Barati. Metall. Mater. Trans. B, 45 (1) (2014) 221-228.
[3] J.J. Wu, T. Nonferr. Metal. Soc., 23 (1) (2013) 260-265.
[4] J.J. Wu, Y.L. Li, W.H. Ma, T. Nonferr. Metal. Soc., 24 (4) (2014) 1231-1236.
[5] Z.Z. Xia, J.J. Wu, W.H. Ma, Sep. Purif. Technol., 187 (2017) 25-33.
[6] N. Naomichi, B. Hiroyuki, S. Yasuhiko, K. Yoshiei, Mater. Trans., 45 (3) (2004) 858-864.
[7] J.J. Wu, W.H. Ma, B.J. Jia, B. Yang, D.C. Liu, Y.N. Dai, J. Non-Cryst. Solids., 358 (23) (2012) 3079–3083.
[8] J.J. Wu, W.H. Ma, B. Yang, Y.N. Dai, K. Morita, T. Nonferr. Metal. Soc., 19 (2) (2009) 463-467.
[9] M. Li, T. Utigard, M. Barati, Metall. Mater. Trans. B, 45 (1) (2014) 221-228.
[10] K. Liu, J.J. Wu, W.H. Ma, J. Min. Metall. Sect. B-Metall., 50 (2) (2014) 171-176.
[11] D.P. Tao, Metall. Mater. Trans. B, 45 (1) (2014) 142-149.
[12] D.P. Tao, D. F. Li, B. Yang, Thermochim. Acta, 383 (2002) 45-51.
[13] D.P. Tao, Thermochim. Acta, 363 (2000) 105-113.
[14] S. Cui, M. Paliwal, I.H. Jung, Metall. Mater. Trans. E, 1 (1) (2014) 67-79.
[15] K. Iwata, T. Matsumiya, H. Sawada, K. Kawakami, Acta Mater., 51 (2003) 551-559.
[16] F. Yang, Q. Yu, J.J. Wu, Vacuum, 158 (2018) 24-30.
[17] R. Noguchi, K. Suzuki, F. Tsukihashi, N. Sano, Metall. Mater. Trans. B, 25 (1994) 903-907.
[18] X.M. Yang, J.Y. Li, P.C. Li, Steel Res. Int., 85 (2) (2014) 164-206.
[19] Y.Q. Zhou, J.J. Wu, W.H. Ma, J. Alloy Compd., 751 (2018) 257-265.
[20] T. Miki, K. Morita, N. Sano, Mater. Trans., 40 (10) (1999) 1108-1116.
[21] T. Miki, K. Morita, N. Sano, Metall. Mater. Trans. B, 28 (1997) 861-867.
[22] T. Miki, K. Morita, N. Sano, Metall. Mater. Trans. B, 29 (1998) 1043-1049.
[23] C. W. Bale, E. Belisle, P. Chartrand, Calphad, 33 (2) (2009) 0-311.
[24] H.C. Wang, Y.C. Dong, Metallurgical Industry Press, (2005).
[25] C. Wagner, Thermodynamics of Alloys, Springer, Berlin, Heidelberg, 1952, p. 51.
[26] Y. Tokuda, T. Yoko, ISIJ International, 49 (6) (2009) 777-782.
[27] R. Noguchi, K. Suzuki, K. Tsukihashi, Metall. Mater. Trans. B, 25 (6) (1994) 903-907.
[28] J.J. Wu, K. Liu, X.M. Chen, Silicon, 7 (3) (2015) 253-259.
[29] T. Yoshikawa, K. Morita, Mater. Trans., 46 (6) (2005) 1335-1340.
[30] H. Dalaker, Computer Method. Mater. Sci., 13 (2013) 407-411.

EKSPERIMENTALNO ODREĐIVANJE KOEFICIJENTA AKTIVNOSTI KOMPONENATA U Si-B-Fe I Si-B-Al TROKOMPONENTNIM SISTEMIMA PRI TEMPERATURI OD 1723 K

F. Yang [a, b], Y.-Q. Zhou [b], J.-J. Wu [a, b*], W.-H. Ma [a, b*], Y. Lei [a, b]

[a*] Glavna laboratorija za vakuumsku metalurgiju obojenih metala, provincija Junan, Kunming, Univerzitet za nauku i tehnologiju, Narodna Republika Kina
[b] Fakultet za metalurško i energetsko inženjerstvo, Univerzitet za nauku i tehnologiju, Narodna Republika Kina

Apstrakt

Interakcije među nečistoćama u rastvorima na bazi Si su važni termodinamički parametri za pročišćavanje silicijumskih materijala. Metod ,iste koncentracije' korišćen je za određivanje koeficijenta aktivnosti Fe prema B i Al prema B u silicijumskom rastvoru. Fe i Al su pojedinačno rastvoreni u dvokomponentnom Si-B rastvoru na temperaturi od 1723 K u trajanju od 5 h, 7 h, 9 h i 11 h. Određene su ravnotežne koncentracije Fe, B u Si-B-Fe sistemu i Al, B u Si-B-Al sistemu. Koeficijenti aktivnosti Fe prema B i Al prema B dobijeni su prilagođavanjem podataka o rastvorljivosti B, Fe i Al. Dobijeni su odnosi rastvorljivosti između B i [%Fe] i između B i [%Al]. Uz pomoć SEM i EPMA slika uzoraka otkriveno je da je treća komponenta Fe ili Al dodata dvokomponentnom Si-B rastvoru bila u potpunosti legirana, što dokazuje tačnost rezultata eksperimentalnog određivanja. Analiziran je značaj koeficijent aktivnosti B na odstranjivanje bora iz industrijskog silicijuma.

Ključne reči: *Rastvor na bazi Si; Trokomponentni sistem; Koeficijent aktivnosti; Maksimalna rastvorljivost; Fizička karakterizacija*