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MATHEMATICAL MODEL OF THE DIAGRAM OF THE Fe-Si-B COMPOSITION SYSTEM

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A diagram of the phase composition of the Fe – Si – B system is constructed in the form of elementary triangles of coexisting phases and its mathematical model was created. Its isothermal sections are given in the temperature range of 300 - 2 000 K. The diagram is composed of one-component phases Fe, Si, B, binary compounds Fe_3Si, Fe_2Si, Fe_5Si_3, FeSi, $FeSi_2$, FeB, Fe_2B, SiB_4, SiB_6, SiB_{14}, as well as ternary phases Fe_5SiB_2 and Fe_5Si_2B. To estimate the sizes of crystallization fields, the areas of elementary triangles were calculated, the probability of existence (prevalence) of each compound in the phase space of the diagram was established.

Keywords: Fe – Si – B system, phase, diagram, isothermal section, mathematical model

INTRODUCTION

The diagrams of state, phase composition and physical properties of the Fe – Si – B system are of interest for various sectors of the economy. Primarily for the ferroalloy and steel industry. The basis for the production of various grades of ferrosilicon is the Fe - Si system [1], aluminothermal ferroboron - Fe – B [2], and silicothermal ferroboron - Fe – Si – B [3]. It is also used to create amorphous alloys that have unique physical, mechanical and chemical properties and are gaining wider application in modern industry, especially in high-tech areas, as materials and coatings. It is noted in [4] that a classical example of obtaining an amorphous state upon ultrafast cooling of metal melts is iron-boron alloys, and the addition of silicon to them, the transition to the Fe – Si – B system significantly increases the operational characteristics of the products obtained.

For these processes, the main task is the formation of the necessary phases in the metal or the establishment of undesirable phases for their removal in various ways. In this work, the task is to identify them by plotting a diagram.

Quantification of these phases from the diagram is usually done using the rule of segments (leverage). When considering many options, this method requires, although simple, but time-consuming calculations. In this work, it was decided to facilitate this process by creating a mathematical model of the phase composition diagram of the Fe – Si – B system and its computer program. The method developed by us for the mathematical description of diagrams [5, 6] allows not only determining the phase composition, but also calculating the required chemical composition of the metal planned for smelting using a given phase composition.

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RESEARCH METHODOLOGY

The main method for constructing state diagrams is experimental. But calculated ones are also used, based on the study of the dependence of the free energy of the system on temperature, pressure, concentration of all components in all phases. In this work, to construct a diagram, computer and thermodynamic-diagrammatic methods are used [7, 8]. In fact, the triangulation of the Fe – Si – B system was carried out, the result of which is a diagram in the form of elementary triangles of coexisting phases. For the mathematical description of the phase composition diagram, we used our own balance method [5].

RESEARCH RESULTS AND THEIR ANALYSIS

The Fe – Si – B ternary system is composed of three binary private systems: Fe – Si, Fe – B and Si – B. In the Fe – Si system, the presence of such silicides as Fe_3Si, Fe_5Si_3, FeSi, $FeSi_2$ and Fe_2Si [1]. Iron borides are formed in the Fe – B system [2]. Most researchers are inclined to believe that those in this system are FeB and Fe_2B, the first of which melts congruently, and the second - incongruently. In the Si – B system, B_4Si and B_6Si are considered to be reliably installed. The SiB_n compound indicated in the literature has a wide homogeneity range (n = 10 - 14). For the construction of the diagram, we adopted the SiB_{14} compound [9].

The researchers note that there are three ternary compounds in the Fe – Si – B system. It is believed that these are Fe_5Si_2B, $Fe_{4.7}SiB_2$ and $Fe_2Si_{0.4}B_{0.6}$ or $Fe_{47}Si_{20}B_{10}$, $Fe_{50}Si_{10}B_{20}$ and $Fe_{20}Si_4B_6$ [10]. With slight deviations, the similarity of the chemical composition of compounds from all three groups is obvious. For plotting the diagram, we selected the Fe_5SiB_2 and Fe_5Si_2B compounds, which are most frequently encountered in scientific works on the Fe – Si – B system. The thermodynamic data of all selected double and ternary compounds were used both in the method of thermodynamic - diagrammatic and computer-based diagrams. In the latter case, the “Triangle” subroutine of the “TERRA” complex is applied.

When using the thermodynamic-diagrammatic method [8], it is recommended to apply all compounds found from the reference literature on the composition triangle (Figure 1). This gives an overall picture of the phase structure of the system. Pairwise coexistence of phases was estimated by calculating the change in the Gibbs energy of the corresponding reactions. So, in the quadrangle of $FeSi$ – $FeSi_2$ – FeB – B_4Si substances (Figure 1), the reaction written along its diagonals

$$4FeB + 5FeSi_2 = 9FeSi + B_4Si \qquad (1)$$

flows in the forward direction with $\Delta G_{298.15} = -92.37$ kJ / mol, as a result of which its products were considered coexisting and connected by a straight line in the diagram. Carrying out this procedure with other compounds made it possible to perform a complete triangulation of the system under study with the establishment of 15 elementary triangles of coexisting phases in it (Figure 1).

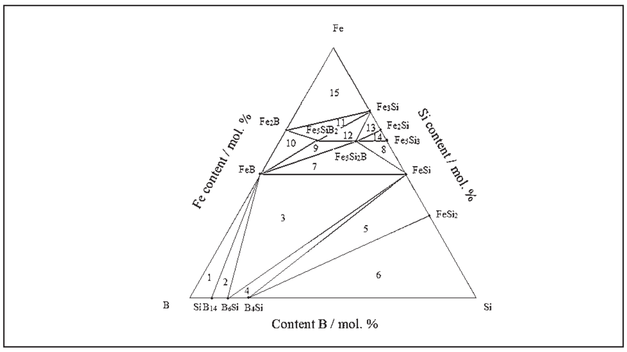

Figure 1 Diagram of the Fe – Si - B system in elementary triangles of coexisting phases.

Table 1 shows the characteristics of the Fe – Si – B system indicating the area of each triangle (S), equations for calculating the amount of the formed phase depending on the chemical composition of the metal under study (Fe_0, Si_0, B_0) and the prevalence of each compound in the phase space of the diagram (W) according to [8].

Table 1 **Characteristics of the Fe – Si – B system**

Triangle No	S /square unit	Equations	Phases	W / %
1	0,01826	$FeB = 2 \cdot Fe_0$ $SiB_{14} = 14{,}925 \cdot Si_0$ $B = -1 \cdot Fe_0 - 13{,}925 \cdot Si_0 + 1 \cdot B_0$	Fe_3Si	5
2	0,01164	$FeB = 2 \cdot Fe_0$ $SiB_{14} = -1{,}881 \cdot Fe_0 - 11{,}276 \cdot Si_0 + 1{,}881 \cdot B_0$ $B_6Si = 0{,}881 \cdot Fe_0 + 12{,}276 \cdot Si_0 - 0{,}881 \cdot B_0$	Fe_2Si	0,47
3	0,10723	$FeB = 1{,}714 \cdot Fe_0 - 1{,}714 \cdot Si_0 + 0{,}286 \cdot B_0$ $B_6Si = -1 \cdot Fe_0 + 1 \cdot Si_0 + 1 \cdot B_0$ $FeSi = 0{,}286 \cdot Fe_0 + 1{,}714 \cdot Si_0 - 0{,}286 \cdot B_0$	Fe_5Si_3	0,69
4	0,01584	$B_6Si = 14{,}035 \cdot Fe_0 - 14{,}035 \cdot Si_0 + 3{,}508 \cdot B_0$ $FeSi = 2 \cdot Fe_0$ $B_4Si = -15{,}035 \cdot Fe_0 + 15{,}035 \cdot Si_0 - 2{,}508 \cdot B_0$	FeSi	19,08
5	0,05592	$FeSi = 3{,}941 \cdot Fe_0 - 1{,}941 \cdot Si_0 + 0{,}485 \cdot B_0$ $B_4Si = 1{,}25 \cdot B_0$ $FeSi_2 = -2{,}941 \cdot Fe_0 + 2{,}941 \cdot Si_0 - 0{,}735 \cdot B_0$	$FeSi_2$	14,82
6	0,11194	$B_4Si = 1{,}25 \cdot B_0$ $FeSi_2 = 3{,}03 \cdot Fe_0$ $Si = -2{,}03 \cdot Fe_0 + 1 \cdot Si_0 - 0{,}25 \cdot B_0$	FeB	16,32
7	0,03044	$FeB = -1 \cdot Fe_0 + 1 \cdot Si_0 + 3 \cdot B_0$ $FeSi = -2 \cdot Fe_0 + 4 \cdot Si_0 + 2 \cdot B_0$ $Fe_5Si_2B = 4 \cdot Fe_0 - 4 \cdot Si_0 - 4 \cdot B_0$	Fe_2B	4,97
8	0,00597	$FeSi = -3 \cdot Fe_0 + 5 \cdot Si_0 + 5 \cdot B_0$ $Fe_5Si_2B = 8 \cdot B_0$ $Fe_5Si_3 = 4 \cdot Fe_0 - 4 \cdot Si_0 - 12 \cdot B_0$	SiB_{14}	2,64
9	0,00685	$Fe_5Si_2B = -4 \cdot Fe_0 + 12 \cdot Si_0 + 4 \cdot B_0$ $Fe_5SiB_2 = 8 \cdot Fe_0 - 16 \cdot Si_0 - 8 \cdot B_0$ $FeB = -3 \cdot Fe_0 + 5 \cdot Si_0 + 5 \cdot B_0$	B_6Si	11,9
10	0,01027	$Fe_5SiB_2 = 8 \cdot Si_0$ $FeB = -1{,}941 \cdot Fe_0 + 1{,}823 \cdot Si_0 + 3{,}941 \cdot B_0$ $Fe_2B = 2{,}941 \cdot Fe_0 - 8{,}823 \cdot Si_0 - 2{,}941 \cdot B_0$	B_4Si	16,23
11	0,00913	$Fe_2B = 2{,}941 \cdot Fe_0 - 8{,}823 \cdot Si_0 - 2{,}941 \cdot B_0$ $Fe_5SiB_2 = -3{,}882 \cdot Fe_0 + 11{,}646 \cdot Si_0 + 7{,}882 \cdot B_0$ $Fe_3Si = 1{,}941 \cdot Fe_0 - 1{,}823 \cdot Si_0 - 3{,}941 \cdot B_0$	Fe_5SiB_2	2,95
12	0,00720	$Fe_5SiB_2 = 2 \cdot Fe_0 - 6 \cdot Si_0 + 2 \cdot B_0$ $Fe_3Si = 3 \cdot Fe_0 - 5 \cdot Si_0 - 5 \cdot B_0$ $Fe_5Si_2B = -4 \cdot Fe_0 + 12 \cdot Si_0 + 4 \cdot B_0$	Fe_5Si_2B	4,92
13	0,00340	$Fe_5SiB_2 = 4 \cdot B_0$ $Fe_3Si = 4{,}125 \cdot Fe_0 - 8{,}375 \cdot Si_0 - 6{,}125 \cdot B_0$ $Fe_2Si = -3{,}125 \cdot Fe_0 + 9{,}375 \cdot Si_0 + 3{,}125 \cdot B_0$		
14	0,00192	$Fe_5SiB_2 = 4 \cdot B_0$ $Fe_2Si = 8{,}333 \cdot Fe_0 - 13{,}888 \cdot Si_0 - 13{,}888 \cdot B_0$ $Fe_5Si_3 = -7{,}333 \cdot Fe_0 + 14{,}888 \cdot Si_0 + 10{,}888 \cdot B_0$		
15	0,03691	$Fe_2B = 3{,}03 * B_0$ $Fe_3Si = 4 * Si_0$ $Fe = 1 * Fe_0 - 3 * Si_0 - 2{,}03 * B_0$		

Table 2 **Compositions of ferroalloys**

No	Alloy	Alloy composition / wt. %					
		Chemical			Phase		
		Fe	Si	B	Si	$FeSi_2$	B_4Si
1	FeSi65	35	65	0	29,79	70,21	0
2	FeSi65B1	36	63	1	26,13	72,22	1,65
3	FeSi65B2	36	62	2	24,48	72,22	3,30

According to the data obtained, the largest area has an elementary triangle B_4Si – $FeSi_2$ – Si, and the smallest - Fe_5Si_2B – Fe_2Si – Fe_5Si_3. In the phase space, iron silicide FeSi has the highest probability of existence (prevalence).

Using the “Triangle” subprogram of the “TERRA” complex, the temperature dependence of the phase composition on temperature was studied, presenting the data obtained in the form of isothermal sections of the diagram. The calculations were performed in the temperature range 300- 2 000 K with a step of 200 K. Some of the results are shown in Figure 2.

The studied system at a temperature of 300K is divided into 8 elementary triangles of coexisting phases. It contains the ternary compound Fe_5SiB_2.

As the temperature rises, changes occur in the composition of condensed phases in accordance with their thermodynamic strength. At a temperature of 1700 K (Figure 2b), stable compounds such as FeSi, FeB, Fe_5SiB_2 and B_6Si are present.

The derived equations (Table 1) allow calculating the phase composition of the metal in the entire space of the Fe – Si – B diagram. Table 2 shows this by the example of FeSi65 ferrosilicon and two grades of boron-containing ferrosilicon.

All alloys are located in the elementary triangle No. 6 B_4Si – $FeSi_2$ – Si, for which the equations are derived (Table 1). In terms of the main components of ferrosilicon, FeSi65 is composed of silicon (Si) and iron disilicide ($FeSi_2$), which were instrumentally found in ingots of industrial metal [1]. The presence of boron in it determines the presence of silicon tetraboride B_4Si as a phase component. If it is necessary to take into account other elements, the same approach is used, since the mathematical model has no restrictions on the number of elements considered in the metal and operates not only in three-dimensional space, where diagrams are usually graphically depicted, but also in multidimensional one.

CONCLUSION

Thus, a diagram of the phase composition of the Fe – Si – B system in the form of elementary triangles of coexisting phases is constructed, its isothermal sections are given, and a mathematical model of the diagram is created that connects the phase composition of the metal with its chemical one. The calculated data are consistent with the results of metallographic studies of industrial metal.

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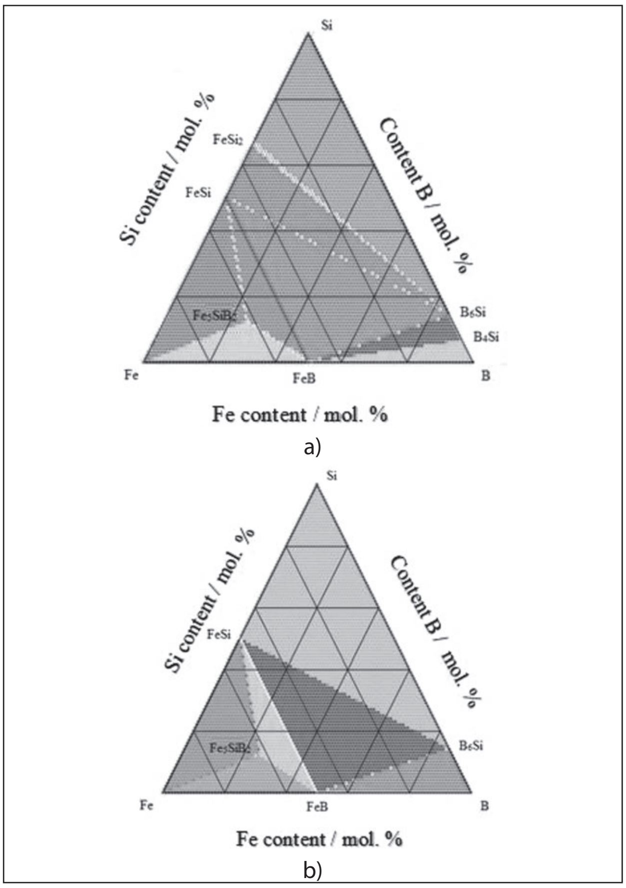

Figure 2 Isothermal sections of the phase composition diagram of the Fe – Si – B system at 300 (a) and 1 700 K (b).

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Note: The responsible translator for English language is Nataliya Drag, Karaganda, Kazakhstan