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DIAGRAM OF EQUILIBRIUM PHASE COMPOSITION OF Fe – C – Si – B SYSTEM

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There has been constructed a diagram of the phase composition of the Fe – C – Si – B system and developed its mathematical model. It permits to determine its phase composition by the chemical composition of the initial material. There is also solved the inverse problem, i.e. the definition of the form and quantity of the initial furnace burden components for obtaining the product of the required phase composition. The analysis established the existence in the studied four-component system of 7 individual phases. There are given examples of using the model for the assessment of the phase composition of metals.

Keywords: Fe – C – Si – B system, phase composition, multicomponent system, compound, mathematical model

INTRODUCTION

Production of industrial and household products is based on development of a certain phase composition in them. In metallurgy, for example, it's achieved by alloying and heat treatment of steel. In the stone casting industry by selection of natural materials in $CaO \cdot MgO \cdot 2\ SiO_2$ diopside crystallization area, and in the production technology of high-temperature ceramics for spark plugs of internal combustion engines by a certain combination of corundum (Al_2O_3), mullite ($3\ Al_2O_3 \cdot 2\ SiO_2$) and calcium hexaaluminate ($CaO \cdot 6\ Al_2O_3$). Under such approach, i.e. goal-oriented development of the phase composition, high quality of finished products can be achieved. For this reason the special attention is paid for search of the optimum phase structure of the products designed to production.

Initial selection of the phase composition is usually made according to the charts of state and physical properties. However, there are certain restrictions. The matter is that it is possible to remove numerical value of any property with a three-component chart, using a four-component is complicated, and five, six or more component is impossible as they can't be correctly shown in a three-dimensional space. We will note that the majority of the charts which are available in literature are three-components, and production furnace charges are multicomponent.

Search of the required phase composition can be introduced by the instrumental control: petrographic, X-ray phase, metallographic. But in case of need to study tens and hundreds of options of stacking for obtaining a product with the required property, instrumental controls will be expensive and longtime. They can't be applied in case of existence of a chemical composition of the raw materials designed to extraction.

It appears that the solution of the task can be facilitated by construction and mathematical description of charts of the phase composition. Developing models remove restrictions by quantity of the components which are present in a product, temperature range, approaching the obtained results to working conditions.

WAYS OF STUDY

In the present work there was defined the aim to construct a diagram of the phase composition of the Fe – C – Si – B system and to develop its mathematical model. A diagram of the phase composition has a special and not similar form to a diagram of the state. It represents a diagram of the coexisting phases. They are joint by straight lines. In this case the diagram of a three - component system represents a set of elementary triangles of the coexisting phases, the 4 - component – tetrahedrons, 5 - component – pentatops, etc.

The method we use to construct a diagram is based on the thermodynamic assessment of the possibility of coexistence of secondary compounds (phases), as well as on the principles of topology of diagrams [1, 2].

The studied four-component Fe – C – Si - B system in graphic representation this diagram represents a tetrahedron including one -, two - and three - component private systems.

In Table 1 there is shown the list of all private systems.

The construction of a diagram of the phase composition of the four - component Fe – C – Si – B system began with private three-component ones (Table 1), re-

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Table 1 **List and number of private systems**

Number		Systems
of components	of systems	
1	4	Fe; C; Si; B
2	6	Fe - B; Fe - C; Fe – Si; B - C; B - Si; C – Si
3	4	Fe –B - C; Fe – B - Si; Fe – C - Si; B – C – Si
4	1	Fe – C – Si – B

vealing in them binary and threefold phases according to the reference data. For constructing the diagram there were used stable (congruently melting) compounds.

The Fe – B – Si system and its fragments have been the subject of several studies [3, 4]. And it is consists of three private binary ones: 1) Fe - B; 2) Fe - Si and 3) B - Si. It is stated that the first time the system has two stable binary compounds FeB and Fe_2B [5] . However by reference data [6, 7] Fe_2B melts with decomposition and charting taken compound FeB .In the second system there is one binary stable compound: FeSi. In the third binary system (B - Si) stable chemical compounds are absent. There are threefold compounds in the system.

The phases were applied on a triangle of compositions (Figure 1). Further the quadrangle of the substances were allocated FeB – Si – B - FeSi and on its diagonals the reaction was written:

$$FeB + Si = FeSi + B \quad (1)$$

Possibility of its behavior was estimated on change of Gibbs energy. For temperatures 273 and 1 873 K it was the following: ΔG_{273} = - 6,534 and ΔG_{1873} = - 3,594 kJ/mol. It means that reaction (1) proceeds in the forward direction, and its products (FeSi and B) are the coexisting phases. For this reason they were connected by a straight line on the chart.

After this for the phase FeB is the only option of coexistence with FeSi. As a result the threefold Fe – Si – B system breaks into three elementary triangles of the coexisting phases: 1) Fe – FeSi – FeB ; 2) FeSi – Si - B; 3) FeSi – B - FeB (Figure 1).

The Fe – C - B system consists of three binary ones: Fe - B, Fe - C and C – B [6, 7]. The Fe - B system was considered above. In the second one there is one binary compound: Fe_3C, and in the third there is also one binary compound: B_4C. The use of the method stated above breaks it into 4 triangles of the coexisting phases (Figure 2): 1) Fe – FeB - Fe_3C, 2) Fe_3C – FeB - C, 3) FeB - B_4C - C, 4) FeB – B - B_4C.

The Fe – Si – C system consists of three private binary ones: 1) Fe - Si; 2) Fe - C and 3) Si - C [6, 7]. After triangulation is breaks into 4 triangles of the coexisting phases (Figure 3): 1) Fe – FeSi - Fe_3C, 2) FeSi – Si - SiC, 3) FeSi – SiC - C, 4) FeSi – C - Fe_3C.

The Si – B - C system was broken into 3 triangles of the coexisting phases (Figure 4): 1) Si – B - SiC, 2) SiC – B - B_4C, 3) SiC - B_4C - C.

The existence of diagrams of the phase composition of private three-component systems permitted to breakdown into elementary tetrahedrons the four - component Fe – C – Si - B system. Beside the used above there were also used the way of “closing” triangles on the tetrahedron by comparison of their compositions [1, 8].

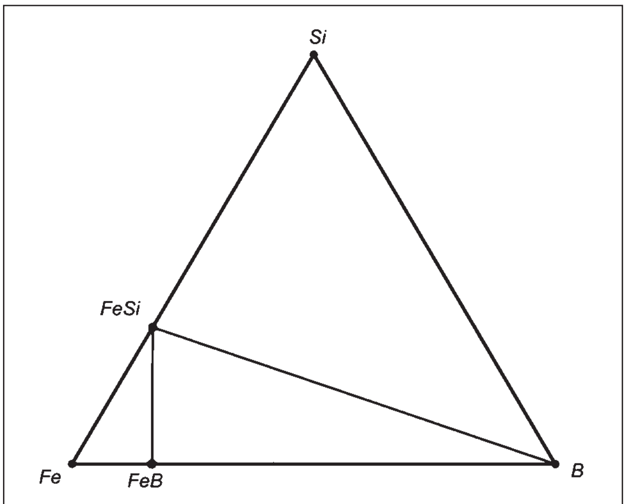

Figure 1 Diagram of the phase composition of the Fe – Si - B system

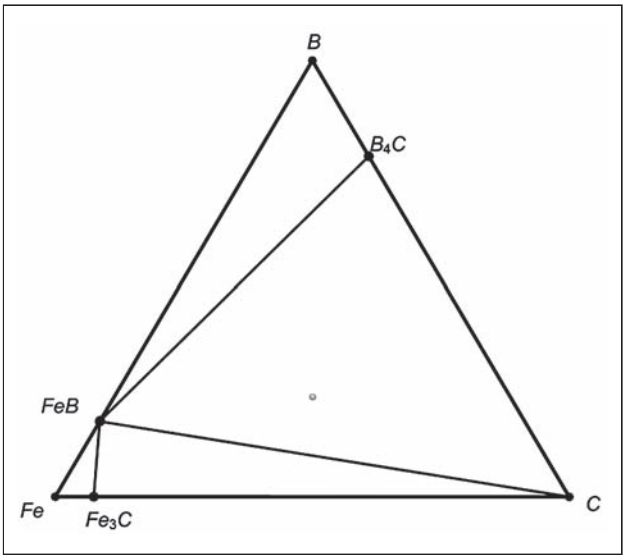

Figure 2 Diagram of the phase composition of the Fe – C - B subsystem

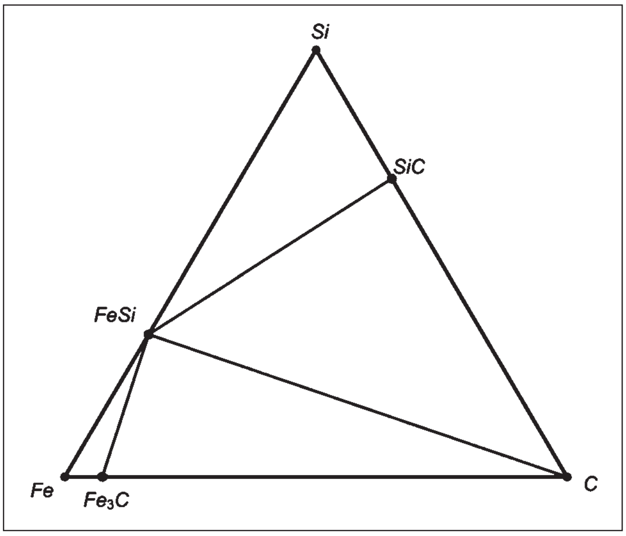

Figure 3 Diagram of the phase composition of the Fe – Si - C subsystem

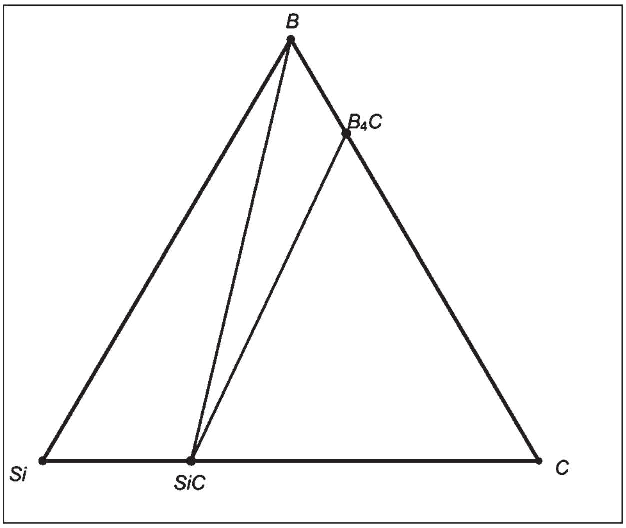

Figure 4 Diagram of the phase composition of the Si – B – C subsystem

It permitted to establish in the Fe – C – Si – B system 7 tetrahedrons of the coexisting phases:

1. Fe - Fe_3C – FeB - FeSi
2. Fe_3C – FeB – FeSi - C
3. FeB – FeSi - B_4C - C
4. FeB – FeSi – B - B_4C
5. FeSi – SiC – C - B_4C
6. SiC - B_4C – B – FeSi
7. FeSi - Si – SiC – B

The graphic representation of the diagram of the phase composition of the Fe – C – Si – B system in elementary tetrahedrons of the coexisting phases is given in Figure 5.

The chart can be used to find the phase composition of metals by geometrical constructions, but to apply this method in a tetrahedron is complicated. Therefore mathematical models for each of 7 elementary tetrahedrons were developed having applied the balance method [9] developed by us. In this method there are made balance equations of initial elements distribution of the alloy by which there are formed phases which solution permits to find expressions for quantitative calculation of phases.

RESULTS AND DISCUSSION

The initial balance and final settlement equations for 7 tetrahedrons are given below. Tetrahedron No. 1 Fe - Fe_3C – FeB - FeSi Through Fe_0, C_0, Si_0 and B_0 were designated the content of iron, carbon, silicon and boron in metal studied according to the chemical analysis.

Balance equations:

B_0=0,1 642 · FeB

C_0= 0,0 667 · Fe_3C

Si_0 = 0,3 333 · FeSi

Fe_0= 1 · Fe + 0,9333 Fe_3C + 0,8 358 · FeB + 0,667

Computational equations:

Fe = Fe_0 – 13,9 925 · C_0- 5,0 901 · B_0 – 2,0003 · Si_0

FeB = 6,0901 · B_0

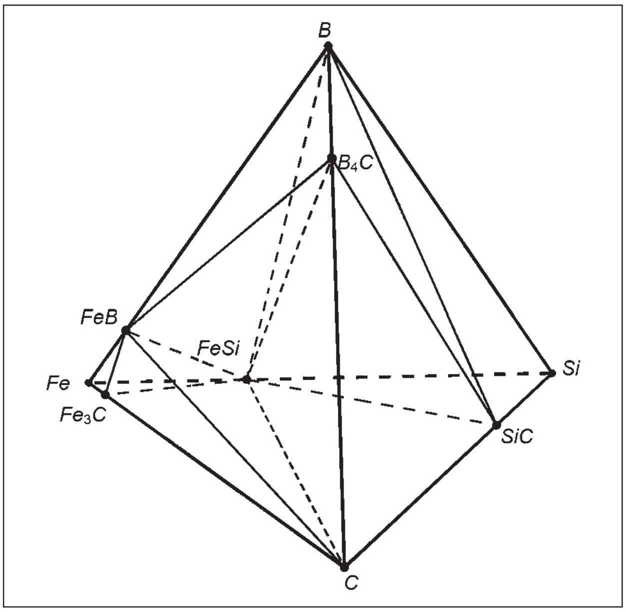

Figure 5 Diagram of the phase composition of the Fe – Si – C - B subsystem

Fe_3C= 14,9 925 · C_0

FeSi = 3,0003 · Si_0

The obtained coefficients at Fe_0, C_0, Si_0 and B_0 in design equations for all tetrahedra were brought to Table 2.

According to the obtained equations, there had been made a computer program that at setting of the chemical composition of the metal (Fe_0, C_0, Si_0, B_0) from the desk switchboard displays its phase composition in weight percentage. The program is exemplified in Table 3. It is seen that commercial ferrosilicon (No.1 and 2) comprises FeSi and Si as phase components, and ferroboron of carbothermal production (No.3) contains FeSi, FeB, B_4C and C. The existence of a mathematical model permits to select a ferroalloy with the phase components required for this or that process. For obtaining high-temperature and wearproof coverings, the metal melting is recommended to be carried out in the diagram fields with the high content of boron carbide (B_4C) (tetrahedrons 3, 4, 5 and 6). For steel alloying the optimum will be tetrahedrons 4, 6 and 7 where boron will have high activity since it is in a free state.

For practical purposes it is important that the obtained models permit to solve both direct and inverse problems of phase formation. For definition of the phase composition of metals by the known chemical composition (a direct problem) there are used computational equations, and for definition of the needed chemical composition of metals (or furnace burden in melting) for obtaining a metal of the set phase composition there are used balance equations derived above.

CONCLUSION

Thus, the diagram of the phase composition of the Fe – C – Si – B system is constructed and its mathematical

Table 2 **Coefficients of equations for calculating the phase compositions**

In.comp.	Coeff.	Coefficients values in tetrahedrons						
		1	2	3	4	5	6	7
		Fe Fe_3C FeB FeSi	Fe_3C FeB FeSi C	FeB FeSi B_4C C	FeB FeSi B B_4C	FeSi SiC C B_4C	SiC B_4C B FeSi	FeSi Si SiC B
C_0	a_1	- 13,9925	1	0	0	0	0	0
	a_2	14,9925	0	0	4,6664	0	0	3,3333
	a_3	0	0	0	0	0	4,6664	0
	a_4	0	0	1	- 3,6664	1	- 3,6664	- 2,3333
S_0	b_1	- 2,0003	0,1430	3,0003	3,0003	0	0	0
	b_2	0	- 2,1433	- 2,3933	0	0	1,4286	0
	b_3	0	0	0,5002	- 2,3933	1,4286	- 2	0
	b_4	3,0003	3,0003	- 0,1072	0,3930	- 0,4286	1,5714	1
F_0	c_1	1	- 1,0715	0	0	1,4999	1,4999	0
	c_2	0	1,0715	1,1965	0	0	- 0,7141	0
	c_3	0	0	- 0,2501	1,1965	- 0,7141	0,9995	1,4999
	c_4	0	0	0,0536	- 0,1965	0,2142	- 0,7853	- 0,4999
B_0	d_1	- 5,0901	0,3638	0	0	0	0	1
	d_2	6,0901	- 5,4539	0	0	1,2728	0	0
	d_3	0	6,0901	1,2728	0	0	0	0
	d_4	0	0	0,2728	1	- 0,2728	1	0

Table 3 Composition of ferroalloys

№	Alloy	The alloy composition, by weight / %										
		Chemistry				Phasic						
		Fe	C	Si	B	SiC	FeSi	FeB	B_4C	B	Si	C
1	FeSi75	25	0	75	0	0	37,5	0	0	0	62,5	0
2	FeSi65	35	0	65	0	0	52,5	0	0	0	47,5	0
3	FeB19(carbon)	78	2,5	0,5	19	0	1,5	92,1	4,9	0	0	1,5

model is developed. It permits to determine its phase composition by the chemical composition of the material. Using the model it is also possible to define the form and quantity of the initial furnace burden for obtaining the product of the required phase composition. Diagrams of metal and oxide systems have an independent value, but they also are an important reference material for thermodynamic modeling of technological processes as it is possible to establish in advance the phase composition of the products of melting, i.e. to fill up the database of the appropriate computer programs.

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