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DIAGRAM OF THE EQUILIBRIUM PHASE COMPOSITION OF THE Fe – Cr – Si – B SYSTEM

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Isothermal sections of the phase composition diagram of the Fe – Si – Cr – B system in the temperature range of 300 – 3 000 K with a step of 200 K are constructed. The diagram is shown at a temperature of 1 900 K, which is typical for silicochromium at the outlet from the furnace. A mathematical model of the diagram has been created in the form of a system of linear equations connecting the chemical composition of the metal with its phase. A computer program has been developed for the numerical calculation of the number of formed phases. Silicochromium with 0,3 – 0,5 % boron is located in the crystallization field $CrSi_2$ – Si – SiB_4 – FeSi.

Keywords: Fe-Si-Cr-B system, phase, diagram, equations, mathematical model

INTRODUCTION

Chromium ores and products made from them are in high demand on the world market. This is due to the possibility of obtaining with their use a wide range of high-quality steels, cast irons, refractories, dyes, bleaches, protective coatings. The undisputed leadership in terms of the consumption of chrome ores belongs to metallurgy. Globally, about 80 % of mined chrome ore is used in metallurgy, 10 % for the production of refractories and the remaining 10 % in the chemical industry. Such a high proportion of the use of chromium in metallurgy is explained by the excellent performance characteristics of chromium-containing steels and alloys. They are obtained using chromium ferroalloys, among which silicochromium and refined ferrochrome deserve special attention, used for smelting stainless, heat-resistant, corrosion-resistant and other critical steel grades. The two-stage method of silicochromium production used in factories has a number of unsolved problems. Often, there is a disturbance in the operation of the furnaces due to the formation of a viscous and refractory slag, which impedes the free exit of metal from the tap hole and leads to the formation of crust on the bottom. Another disadvantage of the two-stage method is the formation of a large number of sublimates under the roof and clogging of gas ducts with them, which makes it necessary to periodically stop the furnaces to remove the deposits. In the production of re-fined ferrochrome grades, silicochromium is used as a reducing agent. This process also has a number of unresolved problems, where, along with a high consumption of charge materials and energy, the resulting slags decompose into a finely dispersed powder that poses a threat to the environment. This work is devoted to the construction and mathematical description of the phase composition diagram of the Fe-Si-Cr-B system. It can be used not only to improve the technology of smelting chromium ferroalloys. The basis for the production of various grades of ferrosilicon is the Fe-Si system [1], aluminum-thermal ferroboron – Fe-B [2], and silicothermal ferroboron-Fe-Si-B [3]. It is also used to create amorphous alloys [4].

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WAYS OF RESEARCH

Phase analysis can be performed using graphically depicted diagrams. If for three-component systems this is done relatively easily, then for multicomponent systems, for example, dimensions four, five or more, this is a difficult and in many cases unsolvable problem. Its solution can be facilitated by creating mathematical models of diagrams, since they allow you to operate not only in three-dimensional space, where diagrams are usually displayed graphically, but also in multidimensional one.

The studied four-component system Fe-Si-Cr-B in the graphic image is a tetrahedron, including one, two and three-component partial systems. Their list is given in Table 1.

The construction of a diagram of the phase composition of a four-component system began with particular three-component systems (Table 1), identifying binary

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

Number		Systems
components	systems	
1	4	Fe; Cr; Si; B
2	6	Fe – Cr; Fe – B; Fe – Si; B – Cr; B – Si; Cr – Si
3	4	Fe – B – Cr; Fe – B – Si; Fe – Cr – Si; B – Cr – Si
4	1	Fe – Si – Cr – B

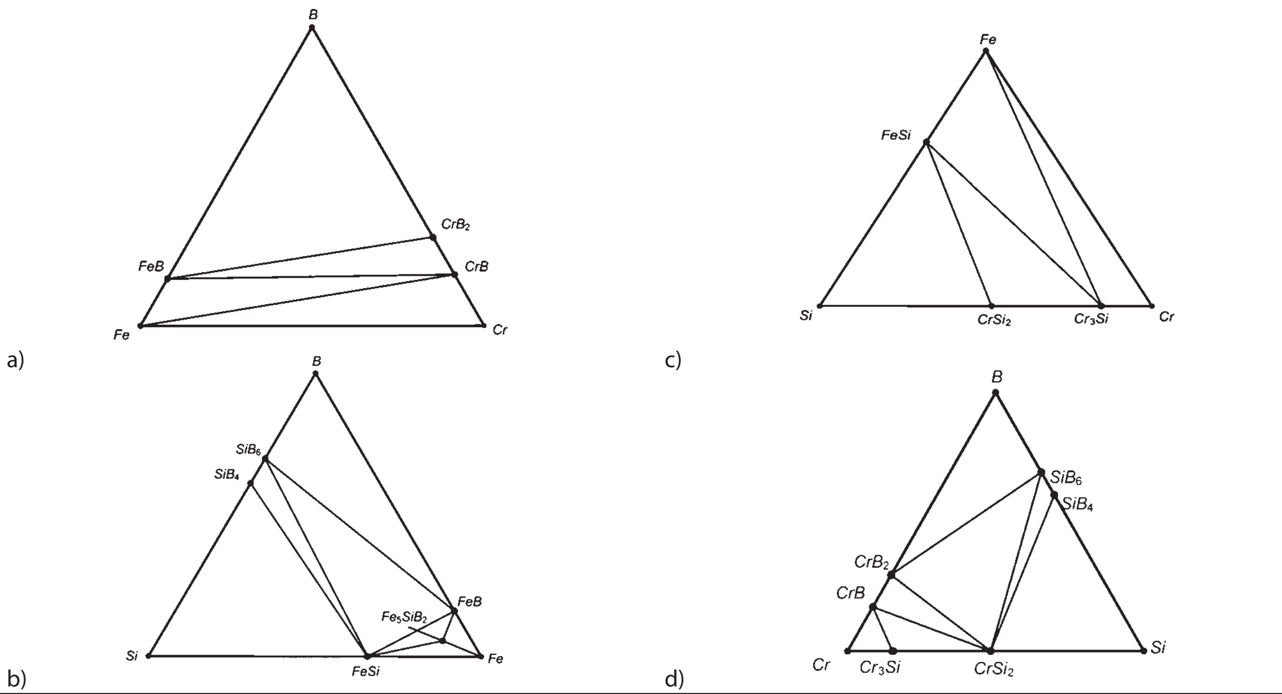

Figure 1 Diagrams of the phase composition of the system (a) Fe – B – Cr, (b) Fe – B – Si, (c) Fe – Cr – Si, (d) B – Cr – Si at 1 900 K

Table 2 **Elementary triangles of the Fe – Si – Cr – B system at 1 900 K**

Triple systems	
Fe – B – Cr	Fe – B – Si
1. Fe – CrB – Cr 2. Fe – CrB – FeB 3. FeB – CrB – CrB_2 4. FeB – B – CrB_2	5. Fe – FeSi – Fe_5SiB_2 6. FeSi – FeB – Fe_5SiB_2 7. FeB – SiB_6 – B 8. SiB_6 – FeB – FeSi 9. SiB_6 – S iB_4 – FeSi 10. SiB_4 – FeSi – Si
Fe – Cr – Si	B – Cr – Si
11. Fe – Cr – Cr_3Si 12. Fe – Cr_3Si – FeSi 13. FeSi – Cr_3S i – $CrSi_2$ 14. FeSi – $CrSi_2$ – Si	15. Cr – CrB – Cr_3Si 16. CrB – Cr_3Si – $CrSi_2$ 17. CrB – CrB_2 – $CrSi_2$ 18. CrB_2 – B – SiB_6 19. CrB_2 – SiB_6 – $CrSi_2$ 20. SiB_6 – SiB_4 – $CrSi_2$ 21. $CrSi_2$ – SiB_4 – Si

and triple phases in them by triangulation using the “Triangle” program of the “Terra” complex [5, 6]. The database of the complex was supplemented with information from reference publications [7]. Isothermal sections of all three-component systems were built in the temperature range of 300 - 3 000 K with a step of 200 K. Below are the data for the characteristic temperature at the outlet of silicon ferroalloys 1 900K (Figure 1).

Table 2 lists all the elementary triangles found after triangulation.

The presence of phase composition diagrams of particular three-component systems made it possible to break down the four-component system Fe-Si-Cr-B into elementary tetrahedrons. We applied the method of “closing” triangles on a tetrahedron by comparing their compositions [8 - 10]. This made it possible to establish that the Fe – Cr – Si – B system has 14 tetrahedra of coexisting phases:

1. Cr – Cr_3Si – CrB – Fe;
2. Fe – FeB – CrB – Fe_5SiB_2;

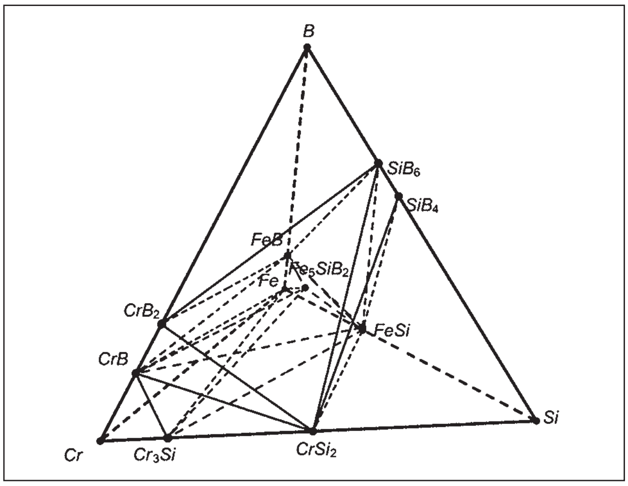

Figure 2 Diagram of the phase composition of the Fe – Cr – Si – B system

3. CrB – Cr_3Si – Fe_5SiB_2 – Fe;
4. Fe – FeSi – Fe_5SiB_2 – Cr_3Si;
5. FeSi – Fe_5SiB_2 – CrB – Cr_3Si;
6. FeSi – FeB – Fe_5SiB_2 – CrB;
7. CrB – CrB_2 – FeB – FeSi;
8. FeB – FeSi – CrB_2 – SiB_6;
9. FeB – B – SiB_6 – CrB_2;
10. Cr_3Si – $CrSi_2$ – CrB – FeSi;
11. CrB – CrB_2 – FeSi – $CrSi_2$;
12. CrB_2 – $CrSi_2$ – SiB_6 – FeSi;
13. SiB_6 – SiB_4 – $CrSi_2$ – FeSi;
14. $CrSi_2$ – Si – SiB_4 – FeSi.

A graphic representation of the diagram of the phase composition of the Fe-Cr-Si-B system in elementary tetrahedra of coexisting phases is given in Figure 2.

The diagram can be used to find the phase composition of metals by geometric constructions, but it is difficult to apply this method in a tetrahedron. Therefore, for each of the 14 elementary tetrahedra, we created mathematical models using the balance method developed by us [11]. In this method, the balance equations for the distribution of the initial alloy elements over the formed phases are first compiled, the subsequent solution of which allows finding expressions for the quantitative calculation of the phases.

RESULTS DISCUSSION

Below, for example, are the initial balance and final design equations for tetrahedron No. 1. In them, Fe_0, Cr_0, Si_0 and B_0 denote the content of iron, chromium, silicon and boron in the studied metal according to chemical analysis.

Balance initial equations:

$Cr_0 = 1 \cdot Cr – 0,85 \cdot Cr_3Si – 0,83 \cdot CrB$

$Si_0 = 0,15 \cdot Cr_3Si$

$B_0 = 0,17 \cdot CrB$

$Fe_0 = 1 \cdot Fe$

Calculated final equations:

$Cr = 1 \cdot Cr_0 – 5,666 \cdot Si_0 – 4,882 \cdot B_0$

$Cr_3Si = 6,666 \cdot Si_0$

$CrB = 5,882 \cdot B_0$

$Fe = 1 \cdot Fe_0$

The coefficients obtained in this way for Fe_0, Cr_0, Si_0 and B_0 in the calculated equations for all tetrahedra were entered in Table 3. Using the obtained equations, a computer program was created, which, when setting the chemical composition of the metal (Fe_0, Cr_0, Si_0 and B_0)

Table 3 **Coefficients of equations for calculating the phase composition**

Ref.	Coeff.	Coefficient values in tetrahedra						
		1	2	3	4	5	6	7
		Cr Cr_3Si CrB Fe	Fe FeB CrB Fe_5SiB_2	CrB Cr_3Si Fe_5SiB_2 Fe	Fe FeSi Fe_5SiB_2 Cr_3Si	FeSi Fe_5SiB_2 CrB Cr_3Si	FeSi FeB Fe_5SiB_2 CrB	CrB CrB_2 FeB FeSi
V		0,025	0,01	0,02	0,2	0,028	0,015	0,037
Cr_0	a_1	1	1,075	0,517	1,176	-0,763	-0,773	2,307
	a_2	0	-1,28	0,671	0	0,593	-2,717	-1,307
	a_3	0		-1,257	-0,519	1,414	3,286	0
	a_4	0	1,205	1,069	0,343	-0,244	1,204	0
S_0	b_1	-5,666	-6,031	-2,934	0	4,328	4,337	-1,99
	b_2	6,666	-5,469	2,865	0	-3,36	2,595	2,36
	b_3	0	12,5	7,127	2,941	-1,351	-5,932	-2,31
	b_4	0	0	-6,058	-1,941	1,383	0	2,94
F_0	c_1	0	1	0	0	-0,714	-0,719	1,026
	c_2	0	0	0	0	1,731	-1,337	-1,216
	c_3	0	0	0	0	0,695	3,056	1,19
	c_4	1	0	1	1	-0,712	0	0
B_0	d_1	-4,882	-5,25	3,353	0	3,728	3,775	-5,384
	d_2	0	6,25	-3,274	14,285	-2,895	13,269	6,384
	d_3	5,882	0	6,14	-3,361	-6,908	-16,044	0
	d_4	0	0	-5,219	-9,924	7,075	0	0
		8	9	10	11	12	13	14
Ref.	Coeff.	Fe FeSi CrB_2 SiB_6	FeB B SiB_6 CrB_2	Cr_3Si $CrSi_2$ CrB FeSi	CrB CrB_2 FeSi $CrSi_2$	CrB_2 $CrSi_2$ SiB_6 FeSi	SiB_6 SiB_4 $CrSi_2$ FeSi	$CrSi_2$ Si SiB_4 FeSi
V		0,167	0,176	0,041	0,044	0,196	0,028	0,193
Cr_0	a_1	-0,366	0	1,405	2,307	1,221	7,342	2,083
	a_2	0,466	-0,428	-0,405	-1,307	0,302	-8,425	-1,083
	a_3	1,428	0	0	0	-0,523	2,083	0
	a_4	-0,528	1,428	0	0	0	0	0
S_0	b_1	-1,993	0	-1,297	-2,13	-1,127	-6,777	0
	b_2	2,538	-2,333	2,297	1,207	1,644	7,777	1
	b_3	0,455	3,333	0	1,923	0,483	0	0
	b_4	0	0	0	0	0	0	0
F_0	c_1	1,027	1,19	0,668	1,096	0,58	3,491	0
	c_2	0,207	-0,19	-1,183	-0,621	-0,847	-4,006	-0,515
	c_3	0	0	0	-0,99	-0,248	0	0
	c_4	-0,234	0	1,515	1,515	1,515	1,515	1,515
B_0	d_1	0,855	0	-6,861	-5,384	0,483	4,333	0
	d_2	-1,088	1	1,979	6,384	-0,704	-3,333	-0,639
	d_3	0	0	5,882	0	1,221	0	1,639
	d_4	1,233	0	0	0	0	0	0

Table 4 **Compositions of ferroalloys**

No	Alloy	Alloy composition / wt. %							
		Chemical				Phase			
		Fe	Cr	Si	B	$CrSi_2$	Si	SiB_4	FeSi
1	FeSiCr48	20	33	47	0	68,7	1	0	30,3
2	FeSiCr 48B0,3	19,7	33	47	0,3	68,7	1,1	0,5	29,7
3	FeSiCr 48B0,5	19,7	33	47	0,5	68,7	1	0,9	29,4
4	FeSiCr 48B0,7	19,7	33	47	0,7	68,7	0,9	1,2	29,2

Table 5 **Probability of the existence of phases**

No.	Phase	W. %	No.	Phase	W. %
1	Fe	0,0605	8	$CrSi_2$	0,1255
2	Si	0,04825	9	CrB	0,055
3	Cr	0,00625	10	CrB_2	0,155
4	B	0,044	11	SiB_6	0,14175
5	FeSi	0,19225	12	SiB_4	0,05525
6	FeB	0,0595	13	Fe_5SiB_2	0,02325
7	Cr_3Si	0,0335			

displays its phase composition in mass percent on the monitor. An example of using the program is shown in Table 4, which presents the phase compositions of conventional and boron-containing ferroalloys calculated using the obtained mathematical models.

All alloys are located in tetrahedron No. 14 $CrSi_2$ – Si – SiB_4 – FeSi. The main phase in silicochromium of the FeSiCr48 brand is $CrSi_2$ and FeSi, boron is a part of SiB_4. Found the volumes (V) of each elementary tetrahedron (table 3). In the phase space of the Fe – Si – Cr – B diagram, the largest volume is occupied by the elementary tetrahedron №14 $CrSi_2$ – Si – SiB_4 – FeSi, and the smallest – №2 Fe – FeB – CrB – Fe_5SiB_2. The operation of the melting furnace in the phase regions of a small volume cannot be recommended due to the possible transition of the metal composition into undesirable fields with inevitable fluctuations in the composition of the charged charge under production conditions.

Determined the probability of the existence of phases W [9] (Table 5).

It can be seen that the phase FeSi, is the most widespread, and Cr is the least widespread.

For practical purposes, it is important that the obtained mathematical models make it possible to solve both direct and inverse problems of phase formation. Calculation equations are used to determine the phase composition of a metal from a known chemical composition (direct problem), and the above-derived balance equations are used to determine the required chemical composition of the metal (or charge into the melt) to obtain a metal of a given phase composition.

CONCLUSION

Thus, a diagram of the phase composition of the 4-component metal system Fe-Si-Cr - B has been constructed. It contains 13 phases: Fe, Si, Cr, B, Cr_3Si, $CrSi_2$, CrB, CrB_2, FeB, FeSi, Fe_5SiB_2, SiB_6 and SiB_4. The sizes of the fields formed and the prevalence of individual phases in them have been determined. The most common phases in the system under study are FeSi, $CrSi_2$, CrB, CrB_2, SiB_4.

A mathematical model of the phase diagram has been created. It allows you to determine the phase composition of the material by the chemical composition. Using the model, it is also possible to determine the type and number of components of the initial charge to obtain a product of the required phase composition.

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