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MATHEMATICAL MODEL OF THE DIAGRAM OF THE PHASE COMPOSITION OF THE SYSTEM Fe – Si – Cr

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Preliminary Note – Prethodno priopćenje

A diagram of the phase composition of the three-component metal system Fe-Si-Cr is plotted. It has 12 phases: Fe, Si, Cr, Fe_3Si, Fe_2Si, Fe_5Si_3, FeSi, $FeSi_2$, Cr_3Si, Cr_5Si_3, CrSi and $CrSi_2$. The dimensions of the fields formed and the prevalence of individual phases in them have been determined. The most common compounds in the system under study are FeSi, $CrSi_2$ and Cr_3Si. Isothermal sections of the diagram are plotted. A mathematical model of the diagram and a computer program have been created. After setting the chemical composition of the metal from the control panel and starting, the computer finds the field (triangle) where the metal is and displays its phase composition in mass percent on a monitor or print. An example of using the created model for calculating the phase composition of ferrosilicon grades is given. FeSi65, FeSi75 and ferrosilicochromium FeSiCr48. A satisfactory agreement was found between the calculated and experimental data.

Keywords: ferroalloy, phase composition, Fe – Si – Cr, diagram, mathematical model

INTRODUCTION

State diagrams are the main tool for creating and analyzing technological processes. With their help, the direction of the processes associated with phase transitions is determined, the choice of heat treatment modes is carried out, the optimal alloy compositions are sought, temperature intervals are assigned during pressure treatment (forging, stamping, rolling, pressing), the melting and pouring temperatures of alloys are determined.

The paper investigates the Fe – Si – Cr system, which describes the production technology of some chromium ferroalloys. It is of particular interest for the production of silicochromium, which is used as a reducing agent in the smelting of refined ferrochrome grades. The production of silicochromium can be compared to the smelting of 45 % ferrosilicon, but this technology uses ferrochrome instead of steel shavings. The latter is the worst solvent for silicon, which causes difficulties in its production. In this work, it was planned to study the features of the formation of metals in the Fe – Si – Cr system by plotting a phase composition diagram to improve the technology for the production of chromium alloys.

RESEARCH METHODOLOGY

The main method for constructing state diagrams is experimental method. 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 [1]. For these purposes, computer programs have been created [2 - 6], widely used in research and production activities [7 - 9]. Their use requires the availability of thermodynamic data for all participants in the process, which is not always possible to ensure. For this reason, along with the computer ("Triangle"), the thermodynamic-diagrammatic method, which has become widespread in research practice [10], is used in this work.

For the mathematical description of the phase composition diagram, we used our own balance method, which differs from the existing ones in simplicity and accuracy in assessing the numerical values of the phases. The use of the described approach makes it possible to remove restrictions on the number of components under consideration, since the mathematical model operates not only in three-dimensional space, where diagrams are usually depicted, but also in multidimensional one.

RESEARCH RESULTS AND THEIR ANALYSIS

The ternary system Fe – Si – Cr is composed of three binary private systems: Fe – Si, Fe – Cr and Si – Cr. The first is characterized by the formation of five iron silicides: Fe_3Si, Fe_2Si, Fe_5Si_3, FeSi, $FeSi_2$. In the Fe – Cr system, no chemical compounds are formed, and in the Cr – Si system there are four chromium silicides Cr_3Si, Cr_5Si_3, CrSi и $CrSi_2$.

According to the recommendation, all found compounds were applied to the composition triangle (Figure 1).

The pairwise coexistence of phases was estimated from the change in the Gibbs energy of the corresponding reactions. For example, in the quadrangle of sub-

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stances Cr – Cr_3Si – Fe – Fe_3Si a chemical reaction written on its diagonal has $\Delta G_{298,15K}$ = – 58,8 kJ / mol.

$$Fe_3Si + 3Cr = 3Fe + Cr_3Si \quad (1)$$

This means its flow in the forward direction and the coexistence of its products. For this reason, they were connected by a straight line in the diagram. As a result, triangle No 1 Fe – Cr – Cr_3Si is formed. Performing this procedure for other compounds made it possible to split the Fe – Si – Cr system into 10 elementary triangles of coexisting phases. A graphic representation of the resulting diagram is given in Figure 1. Thus, 12 phases are installed in the Fe – Si – Cr system: Fe, Si, Cr, Fe_3Si, Fe_2Si, Fe_5Si_3, FeSi, $FeSi_2$, Cr_3Si, Cr_5Si_3, CrSi and $CrSi_2$.

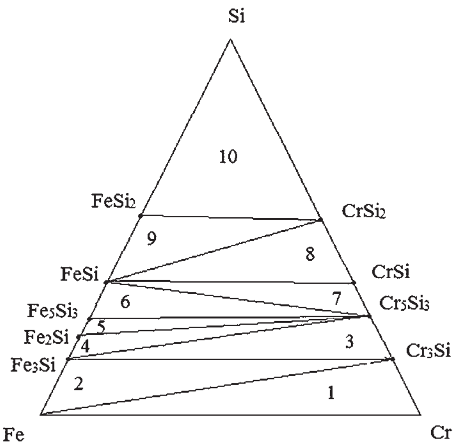

Figure 1 Diagram of the phase composition of the Fe – Si – Cr system in elementary triangles of coexisting phases

Table 1 gives the numbers of all triangles shown in Figure 1, their areas (S), as well as equations found by our own method for calculating the number of phases by the chemical composition (Fe_0, Si_0, Cr_0) of the metal and the probability of the existence of each connections in phase space (W).

The largest size is the triangle Si – $FeSi_2$ – $CrSi_2$, and the smallest one is Fe_5Si_3 – Cr_5Si_3 – FeSi. The operation of the melting unit in the latter cannot be recommended due to the possible transition of the metal composition to the adjacent field with inevitable fluctuations in the flow rate of the charge components in production conditions. The most common phases in the Fe – Si – Cr system are FeSi, $CrSi_2$ and Cr_3Si, forming the melted metal.

A computer program was created using the derived equations. After setting the chemical composition of the metal from the control panel and starting, the computer finds the field (triangle) where the metal is and displays its phase composition in mass percent on a monitor or print.

Table 2 shows an example of using the model to calculate the phase composition of some ferroalloys for the main components.

In ferrosilicon of both grades, the dominant phase is $FeSi_2$, which is close to practical data. For example, in

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

Triangle No	S,square unit	Equations	Phases	W / %
1	0,06432	$Fe = 1 \cdot Fe_0$, $Cr = -5,553 \cdot Si_0 + 1 \cdot Cr_0$ $Cr_3Si = 6,553 \cdot Si_0$	$FeSi_2$	13,27
2	0,05468	$Cr = 0,931 \cdot Fe_0 - 5,553 \cdot Si_0 + 1 \cdot Cr_0$ $Cr_3Si = -1,098 \cdot Fe_0 + 6,553 \cdot Si_0$, $Fe_3Si = 1,167 \cdot Fe_0$	FeSi	13,85
3	0,04120	$Cr_3Si = 1,373 \cdot Fe_0 - 8,19 \cdot Si_0 + 2,655 \cdot Cr_0$ $Fe_3Si = 1,167 \cdot Fe_0$, $Cr_5Si_3 = -1,54 \cdot Fe_0 + 9,19 \cdot Si_0 - 1,655 \cdot Cr_0$	Fe_5Si_3	4,44
4	0,01892	$Fe_3Si = 3,506 \cdot Fe_0 - 13,945 \cdot Si_0 + 4,52 \cdot Cr_0$ $Cr_5Si_3 = 1,324 \cdot Cr_0$ $Fe_2Si = -2,506 \cdot Fe_0 + 14,945 \cdot Si_0 - 4,844 \cdot Cr_0$	Fe_2Si	3,27
5	0,01439	$Fe_5Si_3 = 3,254 \cdot Fe_0 - 6,472 \cdot Si_0 + 2,098 \cdot Cr_0$ $Cr_5Si_3 = 1,324 \cdot Cr_0$ $FeSi = -2,254 \cdot Fe_0 + 7,472 \cdot Si_0 - 2,422 \cdot Cr_0$	Fe_3Si	11,29
6	0,03079	$Fe_5Si_3 = 3,254 \cdot Fe_0 - 6,472 \cdot Si_0 + 2,098 \cdot Cr_0$ $Cr_5Si_3 = 1,324 \cdot Cr_0$ $FeSi = -2,254 \cdot Fe_0 + 7,472 \cdot Si_0 - 2,422 \cdot Cr_0$	$CrSi_2$	17,98
7	0,02609	$Cr_5Si_3 = 3,083 \cdot Fe_0 - 6,131 \cdot Si_0 + 3,311 \cdot Cr_0$ $FeSi = 1,502 \cdot Fe_0$ $CrSi = -3,585 \cdot Fe_0 + 7,131 \cdot Si_0 - 2,311 \cdot Cr_0$	CrSi	7,23
8	0,04743	$FeSi = 1,502 \cdot Fe_0$ $CrSi = 1,433 \cdot Fe_0 - 2,851 \cdot Si_0 + 3,08 \cdot Cr_0$ $CrSi_2 = -1,935 \cdot Fe_0 + 3,851 \cdot Si_0 - 2,08 \cdot Cr_0$	Cr_5Si_3	12,92
9	0,03659	$CrSi_2 = 2,08 \cdot Cr_0$ $FeSi = 3,004 \cdot Fe_0 - 2,986 \cdot Si_0 + 3,226 \cdot Cr_0$ $FeSi_2 = -2,004 \cdot Fe_0 + 3,986 \cdot Si_0 - 4,306 \cdot Cr_0$	Cr_3Si	15,75
10	0,09839	$FeSi_2 = 2,006 \cdot Fe_0$ $CrSi_2 = 2,08 \cdot Cr_0$ $Si = -1,006 \cdot Fe_0 + 1 \cdot Si_0 - 1,08 \cdot Cr_0$		

Table 2 **Compositions of ferroalloys**

N	Alloy	Alloy composition / wt. / %					
		Chemical			Phase		
		Fe	Si	Cr	Si	$FeSi_2$	$CrSi_2$
1	FeSi75	25	75		49,85	50,15	
2	FeSi65	35	65		29,79	70,21	
3	FeSiCr48	10	55	35	7,13	20,06	72,81

it is noted that “dark silicon crystals and a light phase - leboite ($FeSi_{2,3}$), containing aluminum, are revealed in the FeSi75 ingot”. In silicochromium of the FeSiCr48 brand, the main phase component is $CrSi_2$ (Table 2). It was found metallographically in an ingot of the FeSiCrAl alloy [11].

If it is necessary to take into account such impurity elements as Al, C, S, P, the system becomes seven-component. It is not possible to construct it and correctly depict it on a plane. A way out of the situation can be the use of the method of thermodynamic-diagrammatic analysis used in this work and the creation of a mathematical model of the diagram on this basis.

The mathematical model has no restrictions on the number of considered components. To display an *n* - component system, n-1 dimensional space is required, which is provided by a mathematical model. So, to display the 9 and 6 component systems, the 8 and 5 dimensional space was used [12].

Figure 2 shows the isothermal sections of the diagram. At the temperature of the ferrosilicochromium outlet from the furnace (1 900K), the diagram consists of five triangles of coexisting phases: Fe – Cr_3Si – Cr, Fe – Cr_3Si – Fe_3Si, Cr_3Si – Fe_3Si – FeSi, FeSi – Cr_3Si – $CrSi_2$, and at 300K - out of six: Fe – Cr_5Si_3 – Cr, Fe – Cr_5Si_3 – Fe_3Si, Fe_3Si – Cr_5Si_3 – FeSi, Cr_5Si_3 – FeSi – $CrSi_2$, FeSi – $CrSi_2$ – $FeSi_2$, $CrSi_2$ – $FeSi_2$ – Si. It can be seen that not all phases indicated in the complete diagram (Figure 1) are present at these temperatures, which indicates their different thermodynamic stability.

It is important to note that in this system the leading elements (Cr and Si) are bound to form strong chromium and iron silicides, causing their reduced activity. For this reason, ferrosilicochromium is not considered as a strong deoxidizing agent for steel, but is used as a metal reducing agent, for example, in the production of refined ferrochrome.

CONCLUSION

Thus, a diagram of the phase composition of the 3-component metal system Fe – Si – Cr is constructed. It has 12 phases: Fe, Si, Cr, Fe_3Si, Fe_2Si, Fe_5Si_3, FeSi, $FeSi_2$, Cr_3Si, Cr_5Si_3, CrSi and $CrSi_2$. The dimensions 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 $CrSi_2$, FeSi and Cr_3Si. A mathematical model of the diagram and a computer program have been created. After setting the

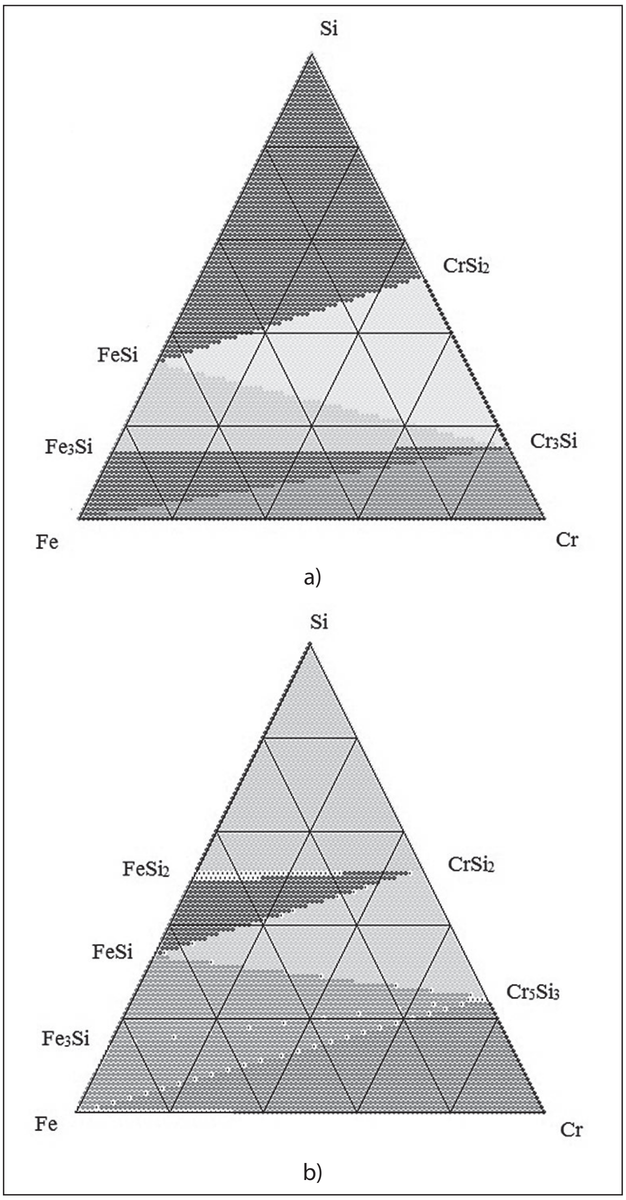

Figure 2 Diagram of the phase composition of the Fe – Si – Cr system at 1 900 (a) and 300 K (b)

chemical composition of the metal from the control panel and starting, the computer finds the field (triangle) where the metal is and displays its phase composition in mass percent on a monitor or print. Isothermal sections of the Fe – Si – Cr diagram are plotted.

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