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THERMODYNAMIC-DIAGRAM ANALYSIS OF THE Fe-Si-Al-Cr SYSTEM WITH THE CONSTRUCTION OF DIAGRAMS OF PHASE RELATIONS

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Preliminary Note – Prethodno priopćenje

The Fe-Cr-Si and Fe-Cr-Al systems are the basic ones in the development of the technology for smelting a new complex alloy - aluminosilicochrome. Aluminosilicochromium can be used as a reducing agent for metallothermic production of low- and medium-carbon ferrochromium grades with subsequent use in the smelting of stainless steel grades. Construction of a diagram of the phase composition of a four-component system Fe-Si-Al-Cr, consisting of 4 three-component systems Fe-Si-Al, Fe-Cr-Si, Fe-Cr-Al, Si-Cr-Al. Three-component Fe-Si-Al system, which will be the base of the Fe-Si-Al-Cr tetrahedron. It is necessary to analyze the thermodynamic properties of compounds for binary and ternary systems.

Keywords: Fe-Si-Al-Cr, phases, thermodynamics diagram, mathematical model.

INTRODUCTION

Industrial alloys refer to systems that occur and exclude metal - the solvent usually occurs in two, three, four, and sometimes more and includes other metals, does not include various impurities. Therefore, the sophistication of new properties and the improvement of the properties of alloys is impossible without knowledge of the many components of the connection diagram. State diagrams of systems are not only informational signals about significant and limited calculated melting indicators, but also about high inflow frequencies for melts close to increased composition indicators, the forecast of the highest temperament, their characteristics and technological modes of production. The generally accepted applications of thermodynamic studies of processes in multicomponent sources are quite complex and require extensive mathematical calculations, including the determination of the thermodynamic values of a large number of significant distributions [1-3].

RESEARCH METHODOLOGY

Analysis of thermodynamic properties of compounds of double state diagrams of the Fe - Cr, Cr - Al, Si - Cr system.

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The state diagram of Fe-Cr is a system with unlimited solubility in both liquid and solid states with a point of equal concentrations. There are no connections in the system.

A minimum is observed on the liquidus and solidus curves at 22 % (at.) Cr and 1 507 °C. Chromium stabilizes o. c. k. modifications of iron and forms with these modifications continuous series of solid solutions. The area of solid solutions of chromium in the city of c. K. modification of iron is relatively narrow and extends to 13,3 % (at.) Cr.

State diagram of Cr-Al. The following incongruent compounds were reliably identified in the system: $CrAl_3$ (T_{melt} = 1 170 °C), $CrAl_4$.

(T_{melt} = 1 011 °C), Cr_2Al_{11} (T_{melt} = 930 °C), $CrAl_7$ (T_{melt} = 725 °C), Cr_5Al_8 (T_{melt} = 890 °C). The congruent compound Cr_2Al has a melting point T_{melt} = 910 °C, which is very low; therefore, none was taken from this system for thermodynamic diagram analysis.

State diagram of Cr-Si [4]. The following compounds are installed in the Cr-Si system: Cr_3Si (congruent, T_{melt} = 1 770 °C), Cr_5Si_3 (congruent, T_{melt} = 1 720 °C), CrSi (incongruent, T_{melt} = 1 475 °C), $CrSi_2$ (congruent, T_{melt} = 1 550 °C).

Three congruent compounds Cr_3Si, Cr_5Si_3, $CrSi_2$ were taken for triangulation.

Fe-Al state diagram. Accepted coordinates (based on the mass fraction) of congruent and incongruent compounds of the Fe-Si-Al-Cr system [5-7].

Thus, congruent metallic compounds in the Fe-Si-Al-Cr system and their coordinates on the quadruple concentration simplex (tetrahedron) have been established.

RESULTS RESEARCH

Tetrahedron of the four-component system Fe - Si - Al - Cr. The state diagram of Fe - Cr - Si is a set of binary compounds formed in its binary systems: Cr - Si, Cr - Fe and Fe - Si. When triangulating the Cr - Fe - Si subsystem, 5 regions were formed:

- Fe - Cr - Cr_3Si;
- Fe - Cr_3Si - Cr_5Si_3;
- Fe-Cr_5Si_3 - FeSi;
- FeSi - Cr_5Si_3 - $CrSi_2$;
- FeSi - $CrSi_2$ - Si.

The state diagram of the Fe - Cr - Al subsystem is a set of binary compounds formed in its binary systems: Cr - Fe, Cr - Al and Fe - Al.

Since we took only one stable congruent Fe_2Al_5 compound for the Fe - Al system, we connect the Cr - Fe_2Al_5 line in accordance with the law of triangulation [8, 9].

As a result of the triangulation of the Fe - Cr - Al subsystem, 2 regions of coexisting phases were established: Fe - Cr - Fe_2Al_5 and Fe_2Al_5 - Cr - Al.

The state diagram of the Al - Cr - Si subsystem is a set of binary compounds formed in its binary systems: Cr - Si, Cr - Al and Si - Al [10-12].

A characteristic feature of this subsystem is that there are stable connections only for the Cr - Si binary system (Appendix D), therefore, according to the law of triangulation, we connect the opposite vertex from congruent connections with a line. As a result, we have 4 regions of coexisting phases:

- Al - Cr - Cr_3Si;
- Al - Cr_3Si - Cr_5Si_3;
- Al - Cr_5Si_3 - $CrSi_2$;
- Al - $CrSi_2$ - Si.

Based on the tetrahedron of four particular three-component systems Fe - Si - Al, Fe - Cr - Al, Fe - Cr - Si and Al - Cr - Si, a diagram of the phase composition of the four-component Fe - Si - Al - Cr system was constructed (Figure 1).

Next, you need to find the elementary tetrahedron that make up this system. There are two methods for constructing a phase composition diagram. The first method is geometric, very difficult for a given tetrahedron due to the large number of phases formed. The list of elementary tetrahedron in the Fe - Si - Al - Cr system is presented in Appendix D. A tetrahedron consists of 24 triangles. In this work, we applied one of the methods for closing a triangle on a tetrahedron. Following this method, six stable tetrahedron were obtained:

- Fe - FeSi - $F_{e2}Al_2Si$ - Cr_5Si_3;
- FeSi - $Fe_3Al_{11}Si_6$ - Si - $CrSi_2$;
- Fe - Cr - Cr_3Si - Al;
- Fe - Cr_3Si - Cr_5Si_3 - Al;
- Al - Cr - Cr_3Si - Fe_2Al_5;
- Fe - Fe_2Al_5 - Fe_2Al_2Si - Cr_3Si.

When connecting the DFS subsystems Fe - Al - Si, Fe - Cr - Si, Fe - Cr - Al, Cr - Al - Si, a tetrahedron of the Fe - Si - Al - Cr system was formed, shown in Figure 1.

Thus, a thermodynamic-diagram analysis of the system Fe - Si - Al - Cr with the construction of diagrams of phase relationships and a mathematical model of its phase structure was created. The diagrams of phase relations of separate parts in the Fe - Si - Al - Cr system are constructed. Triangulation of the Fe - Si - Al - Cr system based on the calculation of the energy of possible reactions (ΔGr_{min}) made it possible to identify a set of stable triangles of coexisting phases with the determination of the main areas of crystallization of aluminosilicochrome for industrial compositions. As a result of the tetrahedron of the analyzed system, it turned out that it consists of 17 elementary tetrahedron.

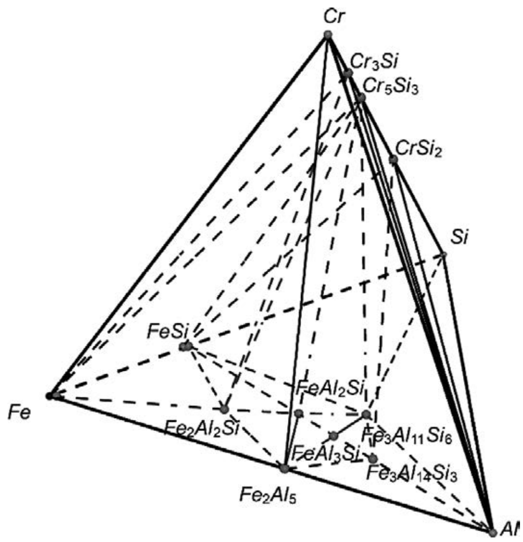

Figure 1 Diagram of the phase structure of the Fe - Si - Al - Cr system [13]

The list of tetrahedron in the Fe - Si - Al - Cr system and their volumes relative to the total volume of the original quaternary system, equal to 1 in arbitrary units show in the Table1.

Table 1 **The list of tetrahedron in the Fe - Si - Al - Cr system**

Tetrahedron	Volume of an elementary tetrahedron, fractions of units
1	2
Si-$Fe_3Al_{11}Si_6$-Fe_2Si_5-$CrSi_2$	0,099264
$FeSi_2$-$Fe_3Al_{11}Si_6$-Fe_2Si_5-$CrSi_2$	0,013536
FeSi-$Fe_3Al_2Si_6$-$FeSi_2$- Cr_5Si_3	0,038352
FeSi-Fe_2Al_2Si-Fe- Cr_5Si_3	0,072072
Fe-Cr_5Si_3-Al-Cr_3Si	0,1
Cr-Fe_2Al_5-Al-Cr_3Si	0,1125
Fe-Cr-Cr_3Si-Al	0,15
$Fe_3Al_{14}Si_3$-Fe_2Al_5-Cr_5Si_3-Al	0,054264
$FeAl_3Si$-$Fe_3Al_{14}Si_3$- Fe_2Al_5-Cr_5Si_3	0,0135789
$FeAl_2Si$-$FeAl_3Si$- Fe_2Al_5- Cr_3Si	0,01445
$FeAl_2Si$-Fe_2Al_2Si- Fe_2Al_5- Cr	0,0228152
Si-$Fe_3Al_{11}Si_6$-Cr_5Si_3-Al	0,2028
FeSi-$FeAl_2Si$-$Fe_3Al_{11}Si_6$-Cr_5Si_3	0,029406
FeSi-Fe_2Al_2Si-$FeAl_2Si$-Cr_5Si_3	0,0289909
$Fe_3Al_{11}Si_6$-$FeAl_2Si$-$FeAl_3Si$-Cr_5Si_3	0,00742014
$Fe_3Al_{11}Si_6$-$FeAl_3Si$-$Fe_3Al_{14}Si$-Cr_5Si_3	0,00736164
$Fe_3Al_{11}Si_6$-$Fe_3Al_{14}Si_3$-Al-Cr_5Si_3	0,026364
Total	1,000000

For each of the tetrahedron, analytical equations are determined, with the help of which it is possible to establish the location in the factor space of the general system of the compositions of various metal melts with the calculation of their normative phase compositions. The breakdown of the overall system was carried out taking into account congruently melting compounds and combining metastable connodes of incongruent components into stable tetrahedron.

CONCLUSION

Thus, a thermodynamic-diagrammatic analysis of the Fe - Si - Al - Cr system was carried out with the construction of diagrams of phase relationships and a mathematical model of its phase structure was created. The diagrams of phase relations of separate parts in the Fe - Si - Al - Cr system are constructed. Triangulation of the Fe - Si - Al - Cr system based on the calculation of the energy of possible reactions (ΔGr_{min}) made it possible to identify a set of stable triangles of coexisting phases with the determination of the main areas of crystallization of aluminosilicochrome for industrial compositions. As a result of the tetrahedron of the analyzed system, it turned out that it consists of 17 elementary tetrahedron. For each of the tetrahedron, analytical equations are determined, with the help of which it is possible to establish the location in the factor space of the general system of the compositions of various metal melts with the calculation of their normative phase compositions. The breakdown of the overall system was carried out taking into account congruently melting compounds and combining metastable connodes of incongruent components into stable tetrahedron. The sum of the relative volumes of elementary tetrahedron is equal to one (1, 000000), which confirms the correctness of the tetrahedron performed. The compositions of the predicted alloys in the region of the Al - Si - $Fe_3Al_{11}Si_6$ - Cr_5Si_3 tetrahedron have been established. Mathematical models for calculating the phase composition of the investigated aluminum-silicochrome alloy are proposed. The sum of the relative volumes of elementary tetrahedron is equal to one (1, 000000), which confirms the correctness of the tetrahedron performed. The compositions of the predicted alloys in the region of the Al - Si - $Fe_3Al_{11}Si_6$ - Cr_5Si_3 tetrahedron have been established.

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