Thermodynamic Analysis of Components Interaction in the System Cr-Fe-Al-O

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ABSTRACT. A complete thermodynamic analysis of the system Cr-Fe-Al-O was carried out for the following compounds:

1. \( \text{Cr}_2\text{O}_3 + 0.5 \text{FeO} + \frac{7}{3} \text{Al} \)
2. \( \text{Cr}_2\text{O}_3 + \text{FeO} + \frac{8}{3} \text{Al} \)
3. \( \text{Cr}_2\text{O}_3 + 1.5 \text{FeO} + 3 \text{Al} \)
4. \( \text{Cr}_2\text{O}_3 + 0.5 \text{FeO} + \frac{14}{3}\text{Al} \)

The basic results for all compounds are presented in the form of diagrams (The dependence of components content on temperature in the temperature range 300-2000K).

Key words: metallic chrome, iron chromite, metallic aluminum, metallic iron.

Alloys of various functional purposes (high-temperature, heat-resistant alloys; resistance for wired elements [1, 2] etc.) are widely used in current technology on the basis of chrome and iron. As a result of this it is interesting to investigate a complete thermodynamic analysis (CTA) of interaction of chrome and iron oxides with aluminum. No information exists about CTA of the indicated process.

The calculations have been done by applying the program Astra 4 [3]. The investigations were conducted at atmosphere pressure of argon (101 kPa) in the temperature range 300-2000 K with step 50°. Moreover, account is taken of condensed (Cr, Fe, Al, FeAl, FeAl', FeAl₂, CrAl₄, Cr₂Al₆, CrFe₂, Fe₂O₃, FeO, Cr₂O₃, Al₂O₃, Al₂O₄, FeAl₂O₄, FeCr₂O₄) and gaseous (Ar, O, O₂, O₃, Cr, Cr₂, CrO, CrO₂, Cr₂O₃, Cr₂O₄, Fe, FeO, FeO₂, Al, Al₂, AlO₂, Al₂O₃, Al₂O₅, Al₂O₇) phases.

A complete thermodynamic analysis of components’ interaction of the system Cr-Fe-Al-O was conducted for the following compounds:

\( \text{Cr}_2\text{O}_3 + 0.5 \text{FeO} + \frac{7}{3} \text{Al} \) (1)
\( \text{Cr}_2\text{O}_3 + \text{FeO} + \frac{8}{3} \text{Al} \) (2)
\( \text{Cr}_2\text{O}_3 + 1.5 \text{FeO} + 3 \text{Al} \) (3)
\( \text{Cr}_2\text{O}_3 + 0.5 \text{FeO} + \frac{14}{3}\text{Al} \) (4)

The basic results of CTA are presented in the form of diagrams (Figs. 1-4). According to Figs. 1-3, interaction of components of the observed system for reaction 1-3 to ~1400 K is characterized by an identical regularity. The difference is only in the quantitative index of products’ reaction.
At ~ 400K the reaction of aluminum with chrome and iron oxides is completed with formation of metallic chrome and iron chromite (CrFe₃). The temperature increase to ~1400 K leads to modulated reduction of CrFe₃ (evidently, at the expense of its decomposition) and, simultaneously, to the occurrence of metallic iron; a maximal quantity is observed at ~1400 K. At the expense of this process, metallic chrome is slightly increased at temperature increase.

In the temperature range ~1400-1450 K, inverse processes of components’ interaction and occurrence of new phases are evident in the system. In particular, a drastic reduction in the quantities of Cr and Al₂O₃ takes place (with the formation of Cr₂O₃ and metallic Al). At the same time: synthesis of a new compound occurs in fusion mixture 1 (reaction 1) – FeAl₂; in fusion mixture 2 (reaction 2) – FeAl₃, Fe₂CrO₄, FeAl₂O₄ and in fusion mixture 3 (reaction 3) – FeAl₂, Fe₂CrO₄, FeAl₂O₄ and FeO. In this temperature range, iron chromite and metallic iron (with the exception of low quantity) practically disappear in fusion mixtures 2 and 3 due to formation of new phases.

Fig. 4, a diagram of components’ interaction of the system, is given for reaction 4, i.e. in the presence of an excess of the reducing agent (Al) in the fusion mixture. It is shown that reduction of chrome and iron oxides by aluminum is completed below ~ 400 K. At this temperature, in addition to chrome, the following products of reduction are formed: CrAl₄ – its quantity increases to ~1000 K, a drastic decrease occurs in the range ~1400-

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**Fig. 1.** Content of components versus temperature for reaction 1: 1 - Al₂O₃; 2 - Fe; 3 - Cr; 4 - CrFe₃; 5 - Cr₂O₃; 6 - FeAl₂

**Fig. 2.** Content of components versus temperature for reaction 2: 1 - Al₂O₃; 2 - Fe; 3 - Cr; 4 - CrFe₃; 5 - Cr₂O₃; 6 - FeAl₂; 7 - Fe₂CrO₄; 8 - FeAl₂O₄

**Fig. 3.** Content of components versus temperature for reaction 3: 1 - Al₂O₃; 2 - Fe; 3 - Cr; 4 - CrFe₃; 5 - Cr₂O₃; 6 - FeAl₂; 7 - Fe₂CrO₄; 8 - FeAl₂O₄; 9 - FeO

**Fig. 4.** Content of components versus temperature for reaction 4: 1 - Al₂O₃; 2 - Fe; 3 - Cr; 4 - CrAl₄; 5 - Cr₂Al₆; 6 - FeAl₂; 7 - FeAl; 8 - Al
1450K and, subsequently, it practically remains constant (2000K); Cr$_3$Al$_4$ – its quantity decreases with the increase of temperature and completely vanishes at ~1150 K; FeAl$_3$ completely vanishes at ~ 1400 K, afterwards, a drastic increase occurs in the range ~1400-1450 K, remaining constant to ~ 2000 K. FeAl increases to ~1400 K and decreases to zero at ~ 1450 K. The occurrence of metallic aluminum and iron takes place at ~ 750 K and 1000K, respectively. Their quantities run up to maximum at ~ 1400 K and completely disappear at ~ 1450 K.

In comparison with the previous three reactions, inverse processes are not observed in the system above ~ 1400 K; this is probably connected with the presence of an excess of reducing agent of the fourth reaction in the fusion mixture (twice as much as the quantity of Al in the fusion mixture of the first reaction).

The composition of metallic alloy at 1400 K for reactions 1-4 is shown in Table (here it is assumed that the elements in the alloy exist in the form of complexes).

<table>
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<th>mass.%</th>
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<td>Fe</td>
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<tr>
<td>1</td>
<td>27.4</td>
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<tr>
<td>2</td>
<td>-</td>
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1. Н.П. Лякишев, М.И. Гасик (1999), Металлургия хрома. М.: ЭЛИЗ, 581 с.

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