THERMODYNAMIC ANALYSIS OF THE Ti-B-O-C SYSTEM

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Keywords: Full thermodynamic analysis, vacuum, oxide, carbothermal reduction.

Complete thermodynamic analysis of the system Ti-B-O-C at atmospheric pressure and in a vacuum for the following structures: 1.TiO_2 - 38.14 wt.%; B_2O_3 - 33.25 wt.%; C - 28.61 wt.%. 2. TiO_2 - 49.07 wt. %; B_2O_3 - 21.40 wt.%; C - 29.53 wt. %. The basic results for all structures are presented in the form of diagrams (dependence of the contents of components on temperature range 700-1800 K)

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INTRODUCTION

Metals and alloys, as well as composite and nanostructural materials, are mainly obtained as a result of different reactions of reduction of oxides, salts and minerals. Because of this investigation of processes of this type was one of the main objectives of theoretical and applied metallurgy.

In recent years, investigations of chemical and phase equilibrium in multicomponent and multiphase systems with the use of modern computer technologies (full thermodynamics analysis – FTA) have intensively developed recently. Of great interest is application of this approach for the obtaining of composite and nanostructure materials.

It should be mentioned that the method of full thermodynamics analysis (FTA), applied by us, allows to judge not only on equilibrium conditions of processes taking place in the system, but also on the mechanism of interaction of components in complex systems, and, consequently, to adjust the composition of the final product.

In this paper, a full thermodynamics analysis (FTA) of carbothermal reduction of oxides TiO_2 and B_2O_3 was carried out at high temperatures in a vacuum for the following compositions:

Table 1. Composition of the studied mixtures, wt. %

Component	Composition 1	Composition 2
TiO_2 -	38.14	49.07
B_2O_3 -	33.25	21.40
C -	28.61.	29.53

Data of FTA of the considered system have not been in the scientific literature. Hence, the results of research of full thermodynamics analysis of this specified system are of great interest. Calculations were carried out using the computer program ASTRA 4, described in Ref.[1] They were accomplished with 50º increment in the temperature range of 500-2000 K.

RESULTS AND DISCUSSION

Among the possible condensed components were considered: C, Ti, TiO, Ti_2O_3, TiO_2, Ti_3O_5, Ti_4O_7, TiC, $TiCO_{0.04}$, $TiC_{0.1}O$, $TiC_{0.4}O_{0.6}$, $TiC_{0.75}O_{0.25}$, B, B_2O_3, B_4C, TiB, TiB_2; and gaseous: O, O_2, O_3, C, C_2, C_3, C_4, C_5, CO, CO_2, C_2O, C_3O_2, Ti, TiO, TiO_2, B, B_2, BO, BO_2, B_2O, B_2O_2, B_2O_3, TiB.

The main results of FTA are presented in the form of charts.

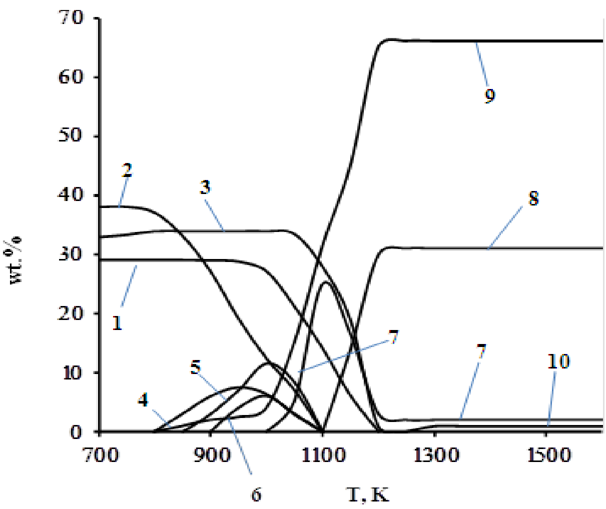

Figure.1 Dependence of the components content on temperature for the Composition 1 in a vacuum: 1–C; 2-TiO_2; 3-B_2O_3; 4-Ti_4O_7; 5-Ti_2O_3; 6-Ti_3O_5; 7–TiC; 8-TiB_2; 9–CO; 10-B_2O_3.

Fig. 1 presents the dependence of the content of components on temperature for the composition 1 in a vacuum (0.0001 atm) in the temperature range of 700-1600 K. It is evident that reduction of TiO_2 begins above 800 K and Ti_2O_3, Ti_3O_5 and Ti_4O_7 are liberated in the condensed phase, amounts of which continue to increase up to ~1000 K, then they decrease and at ~1100 K completely disappear together with TiO_2. Reduction of B_2O_3 starts at ~1000 K, with sharp decrease in its amount and at ~ 1250 K it completely disappears. At ~1000 K separation of TiC begins in the system, its amount drastically increases and at ~1100 K it attains the maximum (~25 wt. %); above this temperature its amount sharply decreases up to ~1250 K to (~1.6 wt. %) and then remains unchanged up to 1600 K. At ~1100 K of TiB_2 starts separating in the system, its amount sharply increases and reaches the maximum (31 wt. %) at ~1250 K; further its amount does not change up to 1600 K. In the gaseous phase emission of CO starts above 800 K (beginning of the process of reduction), the amount of which sharply increases to reach the maximum at about 1250 K, and is not modified further.

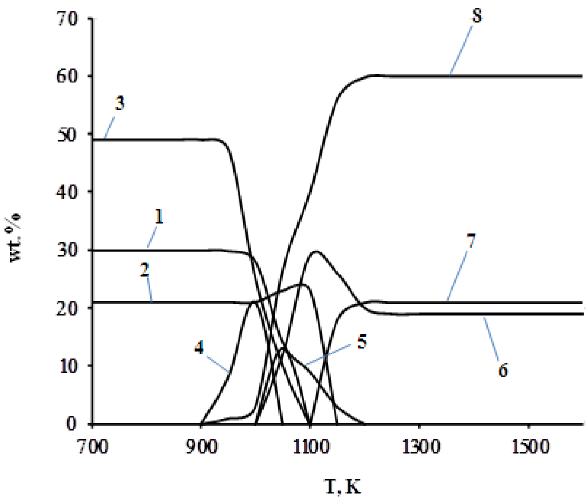

Figure 2. Dependence of the components content on the temperature for the Composition 2 in a vacuum: 1-C; 2-B_2O_3; 3-TiO_2; 4-Ti_4O_7; 5-$TiC_{0.75}O_{0.25}$(c); 6-TiC; 7-TiB_2; 8-CO.

Thermodynamic analysis has shown that for the obtaining of TiB_2 experiments need to take place in a vacuum above 1250 K.

Fig. 2 presents the dependence of the content of components on the temperature for the composition 2 in the temperature interval 700-1600 K in a vacuum (0.0001 atm.).

It can be seen that the reduction of TiO_2 begins above 900K and $TiC_{0.75}O_{0.25}$, Ti_4O_7 are separated in the condensed phase, which quantities increase respectively to ~ 1000 and 1050 K, then decrease, and at about 1100 K all oxides completely disappear. Reduction in the amount of condensed carbon, and parallel to this emission of CO in the gaseous phase, begins above 900 K; starting from 1200 K the condensed carbon disappears in the system and the amount of CO reaches the maximum at ~1200 K and does not change further. From ~1000 K liberation of TiC begins in the system, its amount sharply increases up to 1100K, reaches the maximum (~29 wt. %), then decreases to ~1200 K and above this temperature does not change up to 1600 K (~18 wt. %).

Thermodynamics analysis has shown that in order to obtain the mix of TiB_2 and TiC the experiments need to take place in a vacuum above 1200 K.

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Received: 25.01.2015.
Accepted: 09.03.2015.