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Thermodynamic Analysis of the Ti-B-O-C System and Obtaining of the Mixture of a Boride and Carbide of the Titanium

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ABSTRACT: *The full thermodynamic analysis of the Ti-B-O-C system in vacuum for the following compositions is carried out: 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 main results for all compositions are presented in the form of charts (dependence of the contents of components on temperature in the range of 700-1600 K). On the basis of this analysis is carried out experimental researches on receiving composite materials.*

Keywords: *Boride, Carbide, Carbothermal restoration, Thermodynamic analysis, Vacuum.*

I. INTRODUCTION

At this stage of development of the industry composite nanostructure materials are widely used. Among them it should be noted the materials containing carbides and borides of metals. However their receiving by chemical methods, in particular, recovery processes, requires carrying out broad and careful theoretical and applied research works.

In recent years researches of chemical and phase equilibrium in multicomponent and multiphase systems with use of modern computer [1-2] gained intensive development. Application of this approach for studying of processes of receiving composite and nanostructure materials represents a great interest. It should be noted, that the method of the full thermodynamic analysis used by us – FTA (full thermodynamic analysis) [1] gives the chance to judge not only equilibrium conditions of the processes proceeding in system, but also the mechanism of interaction of components in difficult systems and therefore, to correct structure of the final product. In the work presented by us the task of carrying out the thermodynamic analysis of process of receiving carbides and boride of the titanium and on the basis of this analysis carrying out experimental researches on receiving nanostructure composite materials is set.Innovation of the work is studying of physical and chemical bases of high-temperature processes of receiving carbides and borides of the specified systems that will give the chance of carrying out the minimum quantity of experiments. In present work FTA of carbothermal restoration of TiO_2 and B_2O_3 oxides at high temperatures with formation of carbide and boride of the titan in vacuum for the following compositions**:**

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

Component	**Composition 1 wt.%**	**Composition 2wt.%**
TiO_2	38.14	49.07
B_2O_3	33.25	21.40
C	28.61	29.33

Data on FTA of the considered system in literature aren't found by us. Therefore the great interest represents its carrying out for the specified system. Calculations are carried out on the computer with application of the ASTRA-4 program described in Ref. [1].

They were accomplished with 50^0 C increment in the temperature range of 500-2000 K.

II. 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; 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.

At an research of balance of reaction knowledge of the properties and exact, reliable thermo-dynamic data participating in system of components and connections is necessary. However data on some thermodynamic characteristics of the specified oxycarbides (**□H_{298}, $T_{m.}$, □ $H_{m.}$, C_p, $C_{p\,(l.)}$**) in reference books aren't observed.
In this regard we calculated values of thermodynamic constants of oxycarbides which methods of calculations are developed in work [3] and are brought in a data bank of the **ASTRA-4** program.
The main results of **FTA** are presented in the form of diagrams.**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 restoration of TiO2 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, and further decrease and at ~ 1100 K completely disappear together with TiO_2. Restoration of B_2O_3 starts at ~ 1000 K with sharp decrease of its quantity and at ~ 1250 K it completely disappears. In the system at ~1000K TiC begins to be allocated, its amount drastically increases and at ~1100K 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 1600K. At ~1100 K of TiB_2 starts separating in the system, its amount sharply increases and reaches the maxi-mum (31 wt. %) at ~1250 K; further its quantity doesn't change to 1600 K. In a gas phase higher than 800 K begin allocation of CO (the beginning of process of restoration) which quantity sharply increases and reaches a maximum at ~ 1250 K, and further doesn't change to 1600 K.The thermodynamic analysis showed that for receiving TiB_2 it is necessary to make experiments in vacuum higher than 1250 K.

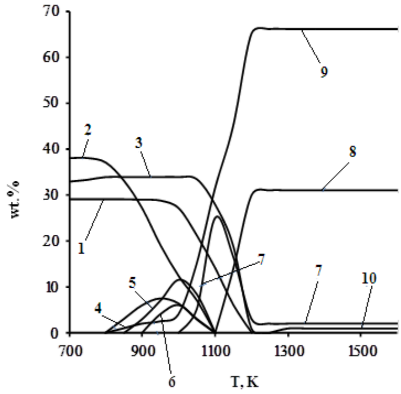

Figure. 1 Dependence of the components content on temperature for the composition1 in a vacuum:

1 - C(c), 2 - TiO_2(c), 3 - B_2O_3(c), 4 - Ti_4O_7(c), 5 - Ti_2O_3(c), 6 - Ti_3O_5(c), 7 – TiC(c), 8 - TiB_2(c), 9 – CO(g), 10- B_2O_3(g).
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 is visible that the restoration of TiO_2 begins higher than 900 K and Ti_2O_3, Ti_3O_5, Ti_4O_7 are allocated in the condensed phase, which quantities increase to ~ 1000 K, and decrease further and at ~ 1100 K all oxides completely disappear. Reduction in the amount of condensed carbon and simultaneous separation in the gaseous phase CO begins higher than 900 K; starting from 1200 K the condensed carbon disappears in the system and the quantity of CO at ~ 1200 K reaches a maximum, and further doesn't change. From ~1000 K liberation of TiC begins in the system, its amount sharply increases up to 1100K, reaches the maximum (~29 wt. %), and decreases further to ~ 1200 K and above this temperature does not change up to 1600 K(~ 18 wt. %).

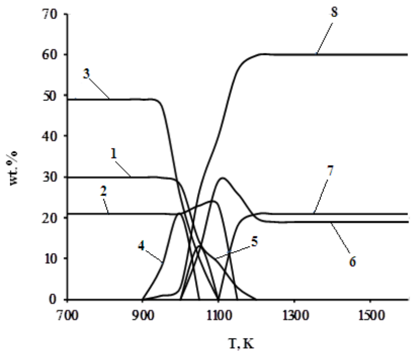

Figure. 2 Dependence of the components content on the temperature for the composition2 in a vacuum:

1 – C(c); 2 - TiO_2(c); 3 - B_2O_3(c); 4 - Ti_4O_7(c); 5 – CO(g); 6 - Ti_2O_3(c); 7 - Ti_3O_5(c); 8 – TiC(c);
9 - TiB_2 (c).

The thermodynamic analysis showed that for receiving the mix TiB_2/TiC it is necessary to make experiments in vacuum higher than 1200 K.

III. EXPERIMENTAL WORK

Proceeding from thermodynamic calculations, for receiving the mix TiB_2/TiC has been taken mix TiO_2, B_2O_3 with graphite which was processed on projected and mounted by us in a mill of high energy (1000 rpm) during 30 hours was taken. The received powder after briquetting it was processed in the high-temperature furnace in the atmosphere of argon at ~ 1400^0C within 3 hours. **Figure 3** presents roentgenogram of the received powder, where it is shown that mix generally turns out TiB2 and TiC; their ratio approximately equals 50-50%.

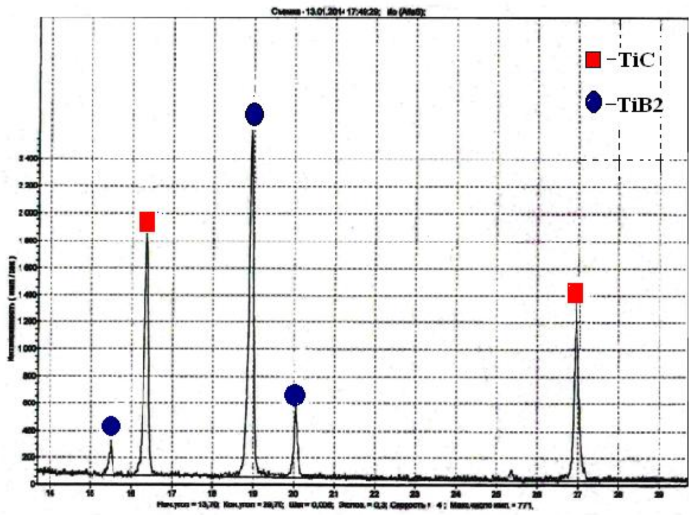

Figure 3. Roentgenogram of TiB_2 /TiC mix

IV. CONCLUSION

1. In the work, the thermodynamics analysis of carbothermal restoration of oxides TiO_2 and B_2O_3 was carried out at high temperatures in a vacuum.
2. It is received mix carbide and boride of the titanium, that it is proved by the X-ray crystallography analysis.

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