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Physical Chemistry

Thermodynamic Analysis of Interaction of B_2O_3 with Carbon

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(Presented by Academy Member Givi Tsintsadze)

ABSTRACT. The work presents full thermodynamic analysis (FTA) of the B-O-C system at atmospheric pressure and in vacuum for the reaction $2B_2O_3 + 7C = B_4C+6CO$. The main results of FTA are plotted in graphs. Comparative analysis of the obtained results shows that carbon reduction of B_2O_3 occurs at much higher temperature at atmospheric pressure than similar processes conducted in vacuum.

Key words: *Full thermodynamic analysis (FTA), boron carbide, vacuum, atmospheric pressure.*

Production of composite and nanostructural materials in most cases is realized through the reactions connected with reduction of oxides. Study of the processes of this type is one of the main tasks of theoretical and applied metallurgy.

Recent years are marked with intensive development of the research of chemical and phase equilibrium in multicomponent and multiphase systems with the use of computer simulation technique (full thermodynamic analysis – FTA) [1–2]. In particular, great is the interest toward applying this approach [1] to study the processes of producing composite and nanostructured materials.

It should be noted that the proposed method (FTA) gives an opportunity to control not only equilibrium conditions of the proceeding processes in the system, but also the mechanism of interaction of components in complicated systems, and to correct the structure of a final product.

The paper presents full thermodynamic analysis (FTA) [1] of interaction of B_2O_3 with carbon at atmospheric pressure and in vacuum. The data on FTA of the considered system have not been found in the appropriate literature. Hence, the results of research of this specified system are of great interest.

Materials and Method

Initial compositions of the investigated system are in compliance with stoichiometry of the following reaction:

$$2B_2O_3 + 7C = B_4C+6CO.$$

Among the possible condensed components: C, B, B_2O_3, B_4C were considered among gaseous ones - O, O_2, O_3, B, B_2, BO, BO_2, B_2O, B_2O_3, C, C_2, C_3, C_4, C_5, CO, CO_2, C_2O, C_3O_2.

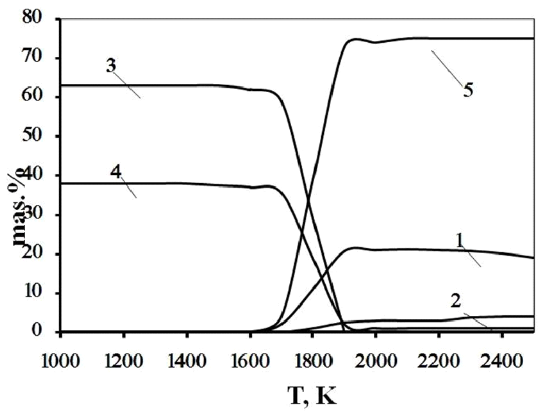

Fig. 1. Temperature dependence of the content of components at atmospheric pressure for the reaction: 1 – B_4C(c), 2-B(c), 3 – B_2O_3(c), 4 – C(c), 5 – CO(g).

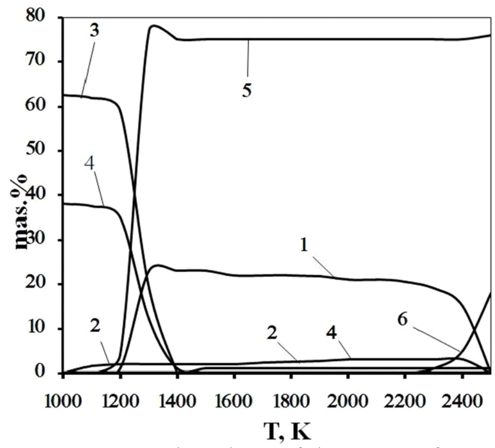

Fig. 2. Temperature dependence of the content of components in vacuum (0,0001atm) for the reaction: 1 – B_4C (c), 2 – B(c), 3 – B_2O_3(c), 4 – C(c), 5 – CO(g), 6 – B(g)

The main results of FTA have been plotted in graphs.

Fig. 1 shows the results of FTA at general atmospheric pressure. Reduction is observed above ~ 1600 K with formation of boron carbide (B_4C), the content of which increases up to ~ 1900 K reaching the maximum at ~ 21 mass %; above this temperature the content of boron carbide slightly changes. The content of condensed B_2O_3 sharply decreases starting from ~ 1600 K and at ~ 1900 K completely disappears.

The content of condensed carbon sharply decreases starting from ~ 1600 K and at ~ 1900 K it reaches 1 mass %; above this temperature it is constant. Condensed boron (~ 3-4 mass%) is precipitated in the system above ~ 1700 K.

Fig. 1 also shows traces of CO appearing in gaseous phase at ~ 1600 K and sharply increasing up to ~ 2000 K; above this temperature CO remains constant allowing us to assume that the process of reduction comes to an end at ~ 2000 K.

Fig. 2 presents TA of the reaction (1) in vacuum (~ $1{,}33\cdot10^{-6}$ MPa) within the temperature range of 1000-2500 K. Reduction of B_2O_3 starts at ~ 1150 K; content of B_2O_3 in the system decreases with the temperature increase and at ~ 1300 K completely disappears. Simultaneously, precipitation of B_4C in the system starts at ~ 1150 K; its content sharply increases to ~ 1300 K and remains constant up to ~ 2000 K. Above this temperature the content of B_4C decreases and at ~ 2500 K completely disappears. The content of condensed carbon sharply decreases starting from ~ 1150 K and at ~ 1300 K reaches 1 mass %; above this temperature the content of carbon remains unchanged. Condensed boron (~ 3-4 mass%) is precipitated in the system above ~ 1250 K.

Fig. 2 also shows the existence of CO in gaseous phase detected at ~ 1150 K; content of the gaseous phase sharply increases to ~ 1300 K and above this temperature remains constant.

Hence, we assume that the process of reduction comes to an end at ~ 1300 K. Above ~ 2000 K boron is released in a gaseous phase; content of boron sharply increases and at ~ 2500 K reaches ~ 18 mass %.

Comparing the results of thermodynamic analysis of the reduction processes we can conclude that carbon reduction of B_2O_3 occurs at much higher temperatures (~1600 K) at atmospheric pressure than similar processes conducted in vacuum (~1150 K): B_2O_3 disappears in the system at ~1900 K and at ~1300 K, respectively. In both cases, reduction starts with the precipitation of B_4C. Precipitation of boron in gaseous phase in vacuum starts at ~2000 K and at ~2500 K its content reaches 18 mass %.

ფიზიკური ქიმია

B_2O_3-ის ნახშირბადთან ურთიერთქმედების თერმოდინამიკური ანალიზი

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შესრულებულია B-O-C სისტემის სრული თერმოდინამიკური ანალიზი ატმოსფერულ წნევაზე და ვაკუუმში შემდეგი რეაქციისათვის: $2B_2O_3+7C=B_4C+6CO$. ანალიზის ძირითადი შედეგები ყველა შედგენილობისათვის წარმოდგენილია დიაგრამების სახით (კომპონენტების შედგენილობის ტემპერატურისაგან დამოკიდებულება 1000-2300 K ინტერვალში).

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