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CRYSTAL STRUCTURE, MICROHARDNESS AND THERMAL EXPANSION OF TERNARY $TaIr_2B_2$ BORIDE

V.V. Lozanov[1], A.V. Utkin[1], G.A. Letyagin[2], G.V. Romanenko[2], D.M. Polyukhov[2], S.G. Kozlova[3,4], A.T. Titov[5], N.I. Baklanova[1]

[1]*Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, Russia*
E-mail: lozanov.25@yandex.ru
[2]*International Tomography Center SB RAS, Novosibirsk, Russia*
[3]*Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia*
[4]*Belgorod Shukhov State Technological University, Belgorod, Russia*
[5]*Sobolev Institute of Geology and Mineralogy SB RAS, Novosibirsk, Russia*

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The ternary $TaIr_2B_2$ boride was prepared by the reaction between iridium and TaB_2 powders. It was shown that a choice in favor of any crystal structure of $TaIr_2B_2$ boride using only X-ray powder diffraction analysis and single-crystal XRD is rather difficult to make. The DFT calculations were carried out to predict the energetically preferred crystal structure of $TaIr_2B_2$. The ^{11}B solid-state NMR spectrum of $TaIr_2B_2$ was recorded for the first time. A combination of diffraction and spectroscopic methods, as well as theoretical calculations, allowed us to make clear choice in favor of the triclinic space group $P\bar{1}$ for the crystal structure of $TaIr_2B_2$. The Vickers microhardness value for $TaIr_2B_2$ was found to be 17.9±2.3 GPa, and the ternary $TaIr_2B_2$ boride can be considered a hard material. Therefore, the family of hard ternary boride phases got a new member. The coefficients of thermal expansion of $TaIr_2B_2$ measured by *in situ* high-temperature XRD analysis are independent of temperature along the *a* and *b* axes, but the CTE along the *c* axis deviates noticeably at elevated temperatures. The findings for the new ternary $TaIr_2B_2$ boride are of interest for the rational design of complex structural materials containing Ta—Ir—B-based components and prediction of their high-temperature behavior. Further research into this ternary boride as well as other iridium-containing ternary borides will provide a tool to solve the problems faced by high-temperature materials science.

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INTRODUCTION

Transition metal borides have a rather wide range of applications resulting from their refractoriness, hardness, superconductivity, as well as mechanical, magnetic, and optical properties [1]. A variety of properties inherent to transition metal borides are related to the fact that they have a rich crystal chemistry and can form crystal structures ranging from 1D to 3D networks.

The family of ternary borides are characterized by an even greater diversity of «structural–chemical–physical» relations. Among ternary borides, those simultaneously containing early and late transition metals (in particular, platinum-group metals) are of special interest.

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CONCLUSIONS

The ternary $TaIr_2B_2$ boride was prepared by the reaction between iridium and tantalum diboride powders at elevated temperatures. The products were comprehensively characterized by a set of modern analytical techniques, including X-ray powder diffraction and single-crystal XRD, SEM/EDX at different accelerating voltages, DFT calculations, and ^{11}B solid-state MAS NMR spectroscopy. It was shown that a clear choice in favor of the *Cc*, *C*2/*c* or $P\bar{1}$ crystal structure of ternary $TaIr_2B_2$ boride using only the common diffraction methods, including X-ray powder diffraction and single-crystal XRD, is rather difficult to make. The DFT calculations showed that the $P\bar{1}$ and *C*2/*c* crystal structures for $TaIr_2B_2$ compound are energetically more preferred (~10 eV) than the Cc crystal structure, but poorly distinguishable from each other ($\Delta E \sim 0.02$ eV). Additional solid-state NMR studies were conducted to solve this problem. The ^{11}B solid-state NMR spectrum of ternary $TaIr_2B_2$ boride was recorded for the first time. The combination of diffraction, theoretical and spectroscopic methods allowed us to make a clear choice in favor of the triclinic space group $P\bar{1}$ for the crystal structure of the ternary $TaIr_2B_2$ phase.

The Vickers microhardness value for the $TaIr_2B_2$ ternary phase was measured to be 17.9±2.3 GPa. Based on this result, ternary $TaIr_2B_2$ boride can be considered a hard material. This value is also comparable to those previously reported for the ternary Hf—Ir—B phases. Therefore, a new member has been added to the family of hard ternary boride phases. The coefficients of thermal expansion were measured for $TaIr_2B_2$ immediately by *in situ* high-temperature XRD analysis. The CTEs of $TaIr_2B_2$ along the *a* and *b* axes are independent of temperature and equal to $7.3 \cdot 10^{-6}$ K^{-1} and $7.2 \cdot 10^{-6}$ K^{-1}, respectively. The temperature dependence of the CTE along the *c* axis noticeably deviates at elevated temperatures. The CTE of the new $TaIr_2B_2$ ternary boride is close to the values determined by us for hafnium–iridium ternary boride.

Therefore, the findings on the crystal structure, microhardness and thermal expansion of new ternary $TaIr_2B_2$ boride are of interest for rational design of the complex structural materials containing Ta—Ir—B-based components and prediction of their high-temperature behavior. There are grounds for hope that further research into this ternary boride and other ternary borides containing iridium will provide a tool to solve problems faced by the high-temperature materials science.

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Supporting information. The Supporting Information is available: Synthesis, Single crystal data, NMR spectra, Powder XRD patterns and EDX analysis, Thermal expansion of the ternary $TaIr_2B_2$ boride (PDF).

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