Titanium boride equation of state determined by in-situ X-ray diffraction

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Abstract

The equation of state (EOS) of titanium boride, TiB 2, was investigated by in situ X-ray diffraction in a diamond anvil cell and multianvil high-pressure apparatus. The pressure-volume-temperature (P-V-T) data were collected at up to 111 GPa and room temperature for the diamond-anvil cell experiments and at up to 15 GPa and 1300 K for the multianvil experiments. No phase transition was observed through the entire range of experimental conditions. The pressure-volume data at room temperature were fitted using a Vinet EOS to obtain the isothermal bulk modulus, $B_T 0 = 256.7$ GPa, and its pressure derivative, $B'_T 0 = 3.83$. When fitting a thermal EOS using the P-V-T data for the multianvil experiments, we find that $(\partial B_T / \partial T)_V = 0.095$ (GPa/K) and $\alpha_0 = 2.49 \times 10^{-5}$ K$^{-1}$.

Keywords: Materials Science, Condensed Matter Physics

1. Introduction

Boride ceramics are well-known for their high melting temperature, hardness, and good chemical inertness. Titanium diboride, TiB 2, has received considerable attention for applications in cutting tools, electrodes, heater materials, and erosion-resistant substrate coatings obtained by chemical vapor deposition (CVD) [e.g., 1, 2, 3, 4]. TiB 2 is used especially as a heater material under extremely high-pressure and high-temperature conditions. For these applications, it is important to predict
and optimize the thermoelastic and mechanical properties of TiB$_2$ [5]. However, the stability of TiB$_2$ at high pressure and high temperature has not been investigated. Most high-pressure studies have been performed at room temperature [e.g., 6]. It is important to know the stability and thermoelastic properties of TiB$_2$ under extreme conditions for the applications described above.

TiB$_2$ has a hexagonal structure with space group $P6/mmm$, with one titanium atom at the origin and two boron atoms at site 2$d$ $(1/3, 2/3, 1/2)$. The melting point of TiB$_2$ is $\sim 3500$ K, and this structure is stable up to at least 60 GPa [6]. The thermal expansion coefficients of TiB$_2$ have been reported using experimental and theoretical methods [7, 8]. The compressibility (bulk modulus) of TiB$_2$ was found to take values between 236 and 260 GPa [5, 6, 9], which were in general agreement with those predicted by theoretical studies [8, 10, 11, 12, 13].

In the present study, we performed high-pressure and high-temperature experiments to investigate the equation of state (EOS) of TiB$_2$. The experiments were performed using synchrotron radiation X-ray diffraction to determine the cell parameters of TiB$_2$. A diamond anvil cell (DAC) and a multianvil press high-pressure apparatus were used at pressures and temperatures up to 111 GPa and 1300 K, respectively. The high temperature region was investigated by the multianvil press because it was difficult to perform stable heating by the DAC using a laser heating system. In contrast, the advantage of the DAC was to generalize for the region above 20 GPa. Therefore, we used the DAC in the high pressure region. The experimental data from both apparatuses were combined to estimate the EOS of TiB$_2$.

2. Experimental

The starting material was a fine-powdered mixture of TiB$_2$, boron nitride (BN), and periclase (MgO). BN was mixed with the sample to reduce the grain growth of TiB$_2$ during heating. MgO acted as a pressure standard and also reduced the grain growth of each phase. In situ X-ray diffraction experiments were performed using the DAC or multianvil apparatus. The cell parameters of the starting material, TiB$_2$, were $a = 3.023(1)$ Å and $c = 3.234(2)$ Å, whereas the volume was 25.588 (28) Å$^3$.

As described in detail previously [14, 15], a combination of the DAC and the multianvil high-pressure system was used to investigate the high-pressure behavior of TiB$_2$. In the DAC experiments, a symmetric-type cell with 60° conical apertures was used [16]. A powdered sample sandwiched between pellets of NaCl powder was loaded into 50–100 μm diameter holes drilled in rhenium gaskets. NaCl was used as the pressure-transmitting and thermal-insulating material. Powdered MgO was mixed with the starting material to provide an internal pressure marker. The sample was heated by an infrared laser to relax the differential stress in the sample.
chamber after each pressure increment. The heated sample was monitored to estimate the heating temperature by an optical microscope. The estimated temperature was \( \sim 2000 \) K. The typical annealing durations were approximately 5–10 min. It is known that a temperature quench could lead to a significant differential stress in the sample chamber. Therefore, the laser power was gradually decreased without invoking a temperature quench at the end of the heating period.

After annealing, the sample was probed by angle-dispersive X-ray diffraction using the synchrotron beam line AR-NE1A at the High Energy Accelerator Research Organization (KEK) or BL10XU at SPring-8. The incident X-ray beams were monochromatized (\( \sim 0.41 \) Å) and collimated to a diameter of 20–50 \( \mu \)m. The distribution of X-ray beam intensity measured by the transmitted X-ray through the DAC was used to adjust the sample position in the X-ray beam. An imaging plate X-ray data collection system (Rigaku) was used to obtain the angle-dispersive X-ray diffraction patterns. The CeO\(_2\) standard was used to calibrate the X-ray wavelength and the distances between the sample and the detector. The two-dimensional diffraction images collected were integrated with FIT2D software in order to obtain the 1D powder diffraction patterns. The each peak position in the diffraction patterns was determined using a peak-fitting program. The lattice constants and volumes of TiB\(_2\) and MgO were determined using a least-squares fit method. The experimental pressure was estimated from the calculated MgO unit cell volume using the EOS for MgO developed by Dorogokupets and Dewaele [17].

The eight cubic anvils of tungsten carbide (WC) with sides of 22 mm and 4.0-mm truncations were used in our multianvil high-pressure system. The high-pressure apparatus “Max III” was installed on the beam line AR-NE7A at KEK. The multianvil press was combined with an energy-dispersive X-ray diffraction system using a white X-ray (Fig. 1). The widths of both the incident and diffracted X-ray beams were 50 \( \mu \)m. The diffracted X-rays were monitored by a germanium solid-state detector at the diffracted angle (2\( \theta \)) of 6°. A cylindrical graphite and a ZrO\(_2\)

![Fig. 1. Schematic illustration of the multianvil press system combined with the synchrotron X-ray measurement.](image)

The sample in the press was probed via energy-dispersive X-ray diffraction using the synchrotron beam line PF-AR NE7A at KEK, Japan. The beam position in the sample was confirmed using an X-ray camera.
sleeve were used as the heater and the thermal insulation. The experimental details are described elsewhere [18]. The powdered mixture of TiB₂, BN, and MgO was used as the starting material. The temperatures of the sample were monitored by a W3%Re/W25%Re thermocouple. The typical temperature fluctuation during the heating was within ±5 °C. In situ measurements were performed using synchrotron X-rays for 5–15 min at the desired pressure and temperature. The cell volume for TiB₂ under each condition was determined by the X-ray diffraction patterns from the sample. The pressure was determined from the measured unit cell volume of MgO using the EOS for MgO [17]. To minimize non-hydrostatic stress in the sample, the X-ray diffraction patterns were acquired during the course of cooling at the fixed oil pressure. The temperature measurement interval was 200 K from 1300 K to 300 K. After data collection at room temperature, the sample was decompressed to the next desired pressure and a similar cycle of data collection was repeated.

3. Analysis

One of the general forms of EOS for solids is

\[ P(V, T) = P_{st}(V, 300) + P_{th}(V, T). \]  

(1)

\[ P(V, T) \] is the total pressure \( P \) at volume \( V \) and temperature \( T \). On the right side of Eq. (1), the first and second terms are the relationship between pressure and temperature at 300 K, and the thermal pressure, respectively. In this article, we have used the Vinet EOS [19] for the first term of Eq. (1),

\[ P_{st}(V, 300) = 3B T_0 \left( \frac{1 - \left( \frac{V}{V_0} \right)^{1/3} } { \left( \frac{V}{V_0} \right)^{1/3} } \right) \exp \left\{ \frac{3}{2} \left( B T_0 - 1 \right) \left[ 1 - \left( \frac{V}{V_0} \right)^{1/3} \right] \right\}, \]  

(2)

where \( B T_0 \) is the isothermal bulk modulus, and \( B T_0' \) is \( (\partial B_T/\partial P)_T \) at ambient temperature. When the temperature is higher than the Debye temperature, the thermal pressure term, \( P_{th} \), often takes a linear form, \( P_{th} = \alpha BT \Delta T \) [20, 21]. In the case that the dependence on temperature, \( \alpha BT \), is negligible, Anderson et al. [21] yields:

\[ P_{th}(V, T) = \left[ \alpha_0 BT_0 + \left( \frac{\partial BT_0}{\partial T} \right)_V \ln \left( \frac{V_0}{V} \right) \right] (T - 300), \]  

(3)

where \( \alpha_0 \) is the coefficient of the volume thermal expansion at ambient condition, and \( (\partial BT_0/\partial T)_V \) is the temperature derivative of the isothermal bulk modulus at constant volume. Finally, Eq. (1) is expressed as

\[ P(V, T) = 3B T_0 \left( \frac{1 - \left( \frac{V}{V_0} \right)^{1/3} } { \left( \frac{V}{V_0} \right)^{1/3} } \right) \exp \left\{ \frac{3}{2} \left( B T_0 - 1 \right) \left[ 1 - \left( \frac{V}{V_0} \right)^{1/3} \right] \right\} + \left[ \alpha_0 BT_0(V_0) + \left( \frac{\partial BT_0}{\partial T} \right)_V \ln \left( \frac{V_0}{V} \right) \right] (T - 300) \]  

(4)

Eq. (4) was used to fit the \( P-V-T \) data from our experiments.
4. Results

In the case of the DAC experiments, two runs were performed at up to 111 GPa at ambient temperature. The experimental pressure was increased at room temperature, and then X-ray diffraction patterns were measured. The strain broadening of the diffraction peaks was confirmed in the room temperature data. This indicated that the large differential stress was induced in the DAC as the pressure was increased. It is known that the differential stress causes a significant systematic bias in the relationship between pressure and structural properties. Therefore, diffraction patterns including strain broadening are not suitable for the $P$-$V$-$T$ study. In this study, the sample was heated after each change in pressure to release the differential stress accumulated during the compression (Fig. 2a). No structural transition was observed up to 111 GPa, and the volume of TiB$_2$ decreased by 23.0% compared with that at ambient pressure. Effects of pressure on the unit-cell parameters and the volume of TiB$_2$ are shown in Table 1 and Fig. 3. In previous experimental studies [5, 6, 9], pressure-volume measurements were performed at pressures below 60 GPa. It is expected that a wider range of experimental pressure leads to more reliable values of the elastic properties. Fitting of the pressure-volume data yielded bulk modulus values of $B_{T0} = 256.7(\pm7.7)$ GPa and $B'_{T0} = 3.83(\pm0.28)$ for the Vinet EOS [19]. The compression curve calculated from the fitted parameters is shown in Fig. 3.

![Fig. 2. Examples of the X-ray diffraction pattern of the sample.](http://dx.doi.org/10.1016/j.heliyon.2016.e00220)

(a) The diffraction pattern obtained in the DAC experiment at 8 GPa and 300 K. (b) The diffraction pattern obtained in the multianvil press experiment at 15 GPa and 1300 K. Peaks are denoted as follows: T, TiB$_2$; P, MgO; S, sodium chloride. The vertical ticks denote the calculated diffraction peaks of each phase: TiB$_2$, MgO, or NaCl.
To assess the quality of the EOS fitted using pressure-volume data, the relationship between the Eulerian strain ($f = \frac{1}{2} \left( \frac{V_0}{V} \right)^2 - 1$) and the normalized pressure ($F = \frac{P}{3(2f+1)^2}$) is shown in Fig. 4. The $f$-$F$ plot provides an indication of higher order terms, such as $B_{T0}'$ and $B_{T0}''$, which are significant in the EOS. The data points plotted in the $f$-$F$ relation lie on a straight line except in the low-$f$ ($<0.02$) region. This indicates that the experimental data was adequately described by a third-order EOS [22]. Most data are plotted around 250 GPa, and the slope of the $f$-$F$ relation ($>0.02$) is nearly zero, which indicates $B_{T0}'$ is close to 4. These relations in our study agree with the findings that the bulk modulus and its pressure derivative are 256.7 GPa and 3.83, respectively.

In the case of the multianvil press experiments, the pressure and temperature were up to 14.6 GPa and 1300 K. Typical X-ray diffraction pattern of the sample is shown in Fig. 2b. The volumes of TiB$_2$ under various pressure-temperature conditions are given in Table 2 and Fig. 3. The experimental data were fitted to Eq. (4). As the volume change at the ambient pressure was not measured, the volume thermal expansion coefficient, $2.489 \times 10^{-5}$ K$^{-1}$ [7], was used.

### Table 1. Lattice parameters and volumes of TiB$_2$ up to 111 GPa at room temperature.

| P(GPa) | a(Å)     | c(Å)     | Volume (Å$^3$) |
|--------|----------|----------|----------------|
| Run #1 |          |          |                |
| 0.0    | 3.029(2) | 3.230(4) | 25.67(5)       |
| 1.1    | 3.017(2) | 3.198(4) | 25.21(4)       |
| 21.6   | 2.962(2) | 3.120(4) | 23.79(4)       |
| 30.9   | 2.938(1) | 3.097(1) | 23.14(1)       |
| 42.6   | 2.914(1) | 3.062(2) | 22.53(2)       |
| 61.4   | 2.874(1) | 3.016(3) | 21.57(3)       |
| Run #2 |          |          |                |
| 7.8    | 2.997(9) | 3.176(11)| 24.71(18)      |
| 11.6   | 2.985(9) | 3.164(11)| 24.41(17)      |
| 29.0   | 2.937(4) | 3.125(8) | 23.35(9)       |
| 33.9   | 2.926(2) | 3.093(3) | 22.93(3)       |
| 64.8   | 2.874(1) | 2.997(3) | 21.44(3)       |
| 73.8   | 2.856(1) | 2.972(2) | 21.00(2)       |
| 83.0   | 2.840(2) | 2.940(7) | 20.54(5)       |
| 89.5   | 2.820(4) | 2.955(5) | 20.34(7)       |
| 99.8   | 2.808(3) | 2.924(4) | 19.96(4)       |
| 111.0  | 2.792(3) | 2.918(4) | 19.69(5)       |

The X-ray diffraction data were measured at room temperature after annealing. The numbers in parentheses are the error (standard deviation, 1σ) in the lattice parameters and volumes.
Fig. 3. Pressure-volume data for TiB$_2$.
The volume data represented by red squares and blue symbols were acquired by the diamond anvil cell and the multianvil press, respectively. The X-ray diffraction patterns for the DAC were collected at ambient temperature after laser annealing. Those for the multianvil press were collected at 300–1300 K. The dashed line denotes the result of a least-squares fit of the volume data for the DAC experiments. The inset shows the enlargement at low pressures. Temperatures of the multianvil experiments were denoted as follows: circles, 300 and 500 K; triangles, 700 and 900 K; diamonds, 1100 and 1300 K.

Fig. 4. Eulerian strain-normalized pressure (F-f) plot of TiB$_2$.
The dashed line represents the bulk modulus, 256.7 GPa, determined by experimental data. The bars represent the errors of calculated values.
Table 2. Observed lattice parameters and volumes of TiB$_2$ of multianvil press experiments.

| P(GPa) | T(K) | Volume (Å$^3$) | P(GPa) | T(K) | Volume (Å$^3$) |
|-------|------|---------------|-------|------|---------------|
| 0.0   | 300  | 25.59(3)      | 10.2  | 700  | 24.83(11)     |
| 3.7   | 300  | 25.03(3)      | 11.7  | 700  | 24.71(9)      |
| 5.5   | 300  | 24.95(6)      | 12.9  | 700  | 24.62(4)      |
| 7.3   | 300  | 24.82(10)     | 3.8   | 900  | 25.40(9)      |
| 9.0   | 300  | 24.67(12)     | 5.5   | 900  | 25.31(4)      |
| 10.3  | 300  | 24.54(6)      | 7.6   | 900  | 25.14(6)      |
| 11.7  | 300  | 24.47(4)      | 10.8  | 900  | 24.83(11)     |
| 3.6   | 500  | 25.11(7)      | 12.3  | 900  | 24.78(5)      |
| 6.0   | 500  | 25.08(3)      | 13.5  | 900  | 24.70(3)      |
| 7.7   | 500  | 24.91(12)     | 4.5   | 1100 | 25.48(7)      |
| 9.7   | 500  | 24.76(10)     | 5.1   | 1100 | 25.37(3)      |
| 11.0  | 500  | 24.61(9)      | 7.5   | 1100 | 25.22(8)      |
| 12.3  | 500  | 24.54(4)      | 10.9  | 1100 | 25.03(13)     |
| 3.5   | 700  | 25.31(4)      | 12.7  | 1100 | 24.92(5)      |
| 5.6   | 700  | 25.17(5)      | 14.0  | 1100 | 24.82(6)      |
| 7.7   | 700  | 25.01(8)      | 14.6  | 1300 | 24.89(2)      |

The numbers in parentheses are the error (standard deviation, 1σ) in the volumes.

volume of the starting material, 25.588 Å$^3$, was used as the value of $V_0$. When the value of $B_{T_0}'$ was set to $B_{T_0}' = 4$, the isothermal bulk modulus and $(\partial B_{T_0}/\partial T)_V$ were determined to be $B_{T_0} = 214(7)$ GPa and $(\partial B_{T_0}/\partial T)_V = 0.094(24)$ GPa/K, respectively.

5. Discussion

The bulk modulus at ambient temperature determined by the multianvil press experiments was 17% smaller than that determined by the DAC experiments. This discrepancy might be due to the difference in the pressure range between the two methods. It is generally recognized that a wider range of pressures leads to a more reliable value for the bulk modulus. As the pressure range (<111 GPa) for the DAC experiments was several times wider than that (<15 GPa) for the multianvil press experiments, the bulk modulus determined by the DAC is suitable for the EOS of TiB$_2$. Table 3 lists the thermoelastic parameters proposed from the combination of DAC and multianvil press results using the thermal EOS, Eq. (4).

Table 4 shows a comparison of $B_{T_0}$ and $B_{T_0}'$ between our study and previous ones. In the case of the theoretical studies, the values of the bulk modulus were scattered (206 < $B_{T_0}$ < 305 GPa). It is known that the methods of calculation have a
significant effect on the calculated numerical values of elastic properties. For example, Panda and Chandran [11] reported that the bulk modulus of TiB$_2$ from first-principles calculations implementing the Hartree–Fock method was 20% higher than that from calculations implementing of density functional theory. In contrast, the values from the experiments were not scattered (236 < $B_{T0}$ < 260 GPa). The bulk modulus, 256.7 GPa, determined in our study was in general agreement with those reported by previous experimental studies.

The pressure derivative of the bulk modulus, $B_{T0}'$, determined in our study was 3.83, which was consistent with those reported by previous theoretical studies [10, 11]. However, this value was larger than that reported by another experimental study [6]. A possible explanation for the inconsistency in the pressure derivative of the bulk modulus is the difference in stress conditions between previous studies and ours. Amulele et al. [6] performed room temperature compression without the relaxation of the accumulated stress in the sample chamber. The differential stress induced by room temperature compression can have an influence on the

| Parameters          | $B_{T0}$ (GPa) | $B_{T0}'$ | Reference                  |
|---------------------|----------------|-----------|----------------------------|
| Theory              | 292            | 3.34      | Pereira et al. [10]        |
|                     | 249–304        |           | Panda and Chandran [11]    |
|                     | 245            | 3.88      | Peng et al. [12]           |
|                     | 206.7          |           | Shein and Ivanovskii [13]  |
|                     | 247.0          |           | Wang et al. [8]            |
| Experiment          | 240            |           | Munro [5]                  |
|                     | 236.3          | 2.57      | Amulele et al. [6]         |
|                     | 260            |           | Waśkowaka et al. [9]       |
|                     | 256.7          | 3.83      | This study                 |
measurement of elastic properties. In contrast, laser annealing was performed at each pressure change before the measurement of X-ray diffraction data in our study. Another possibility was the difference in experimental technique between our study and previous ones. A pressure-transmitting medium, which might have had an influence on the stress condition in the sample chamber, was not used in previous studies [6]. This might have led to the inconsistency in the value of the pressure derivative of the bulk modulus between our study and previous ones.

Declarations

Author Contribution statement

Shigeaki Ono: Conceived and designed the experiments; performed the experiments; analyzed and interpreted the data; wrote the paper.

Takumi Kikegawa: Performed the experiments; contributed reagents, materials, analysis tools or data.

Competing interest statement

The authors declare no conflict of interest.

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Additional information

No additional information is available for this paper.

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