

Equation of state for titanium boride

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1 Introduction

Boride ceramics are well-known for their high melting temperature, hardness, and good chemical inertness. Titanium diboride, TiB₂, has received considerable attention for applications in cutting tools, electrodes, heater materials, and erosion-resistant substrate coatings obtained by chemical vapor deposition. TiB₂ 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 TiB₂. However, the stability of TiB₂ at high pressure and high temperature has not been investigated. Most high-pressure studies have been performed at room temperature. It is important to know the stability and thermoelastic properties of TiB₂ under extreme conditions for the applications described above.

2 Experiment

The starting material was a fine-powdered mixture of TiB₂, boron nitride (BN), and periclase (MgO). BN was mixed with the sample. MgO acted as a pressure standard. In situ X-ray diffraction experiments were performed using the DAC or multianvil apparatus. The cell parameters of the starting material, TiB₂, were $a = 3.023(1) \text{ \AA}$ and $c = 3.234(2) \text{ \AA}$, whereas the volume was $25.588(28) \text{ \AA}^3$.

As described in detail previously [1,2], a combination of the DAC and the multianvil high-pressure system was used to investigate the high-pressure behavior of TiB₂. In the DAC experiments, 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. The sample was heated by an infrared laser to relax the differential stress in the sample chamber after each pressure increment. After annealing, the sample was probed by angle-dispersive X-ray diffraction using the synchrotron beam line AR-NE1A. The experimental pressure was estimated from the calculated MgO unit cell volume using the EOS for MgO.

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. The multianvil press was combined with an energy-dispersive X-ray diffraction system using a white X-ray. The diffracted X-rays were monitored by a germanium solid-state detector at the diffracted angle (2θ) of 6° . The powdered mixture of TiB₂, BN, and MgO was used as the starting material. The temperatures of the sample were monitored by a W_{3%}Re/W_{25%}Re thermocouple. 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. The temperature measurement interval was 200 K from 1300 K to 300 K.

3 Results and Discussion

In the case of the DAC experiments, two runs were performed at up to 111 GPa at ambient temperature. Fitting of the pressure-volume data yielded bulk modulus values of $B_{T_0} = 256.7(\pm 7.7) \text{ GPa}$ and $B'_{T_0} = 3.83(\pm 0.28)$. In the case of the multianvil press experiments, the pressure and temperature were up to 14.6 GPa and 1300 K. As the volume change at the ambient pressure was not measured, the volume thermal expansion coefficient, $2.489 \times 10^{-5} \text{ K}^{-1}$, was used. The volume of the starting material, 25.588 \AA^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 temperature deviation of bulk modulus were determined to be $214(7) \text{ GPa}$ and $0.094(24) \text{ GPa/K}$, respectively [3].

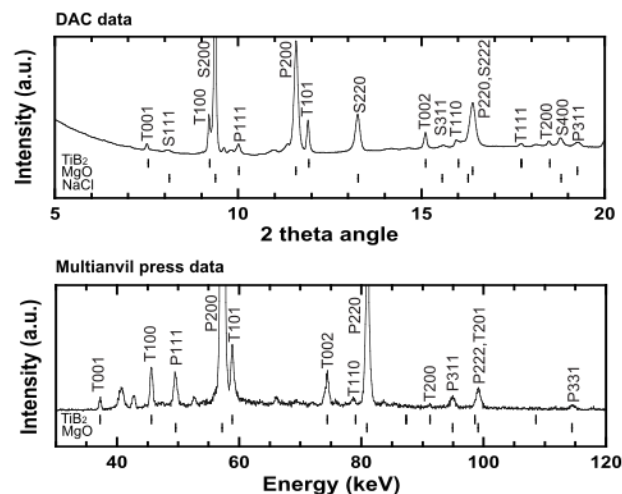


Fig. 1: Examples of the X-ray diffraction pattern of the sample.

References

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