

Mechanical anisotropy and ideal strength of ThBC

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ABSTRACT

The mechanical and thermodynamic properties of ThBC were examined by first-principles calculations based on density functional theory. The equilibrium geometry, elastic stiffness constants, mechanical moduli, Poisson's ratio, elastic wave velocities, and Debye temperature of ThBC were systematically investigated. ThBC exhibits ductile characteristics. The directional Young's modulus E and bulk modulus B and several mechanical anisotropic factors show the mechanical anisotropic properties of ThBC. Under tensile strain, ThBC is easy to cleave along the [111] direction, with an ideal strength of 5.7 GPa. The fracture in ThBC under shear strain occurs along the $[1\bar{1}0]$ direction of the (111) plane. Phonon calculations revealed the thermodynamic stability of ThBC, which is consistent with the experimental observation. The Helmholtz free energy, entropy, and heat capacity were obtained under the quasi-harmonic approximation.

1. Introduction

Actinides have attracted considerable attention from the scientific community given their important applications in the nuclear industry. Thorium and its compounds have received renewed interest in recent years because they are considered potential nuclear fuels for generation IV reactors [1]. A clear understanding of the physical and chemical properties of thorium compounds that are present at various stages of the fuel cycle is crucial to developing the thorium fuel cycle. Therefore, the structural, electronic, and thermodynamic properties of thorium compounds, such as hydrides [2–6], oxides [7–15], carbides [16–25], and nitrides [26–29], have been extensively studied.

Actinide borocarbides possess extremely rich structural diversity and electronic properties that are mainly due to the flexible B–C framework. Boron and carbon atoms can form planar, two-dimensional (2D) networks that alternate with metal atom sheets in actinide borocarbides. Several actinide borocarbides, such as ThB₂C, UB₂C, NpB₂C, and PuB₂C [30], contain these 2D networks. The 2D B–C network of β -UB₂C, ThB₂C, NpB₂C, and PuB₂C is composed of regular (6B) and irregular (6B + 3C) six-membered rings of chemical formula B₆C₃. Carbon atoms occupy the centers of rectangular bipyramids formed by four metal atoms. Another 2D B–C network with an irregular (6B + 2C) six-membered ring exists in low-temperature α -UB₂C. In α -UB₂C, boron and carbon atoms occupy the center points of triangular metal prisms and the centers of rectangular metal bipyramids, respectively [31]. β -UB₂C is found to enter a ferromagnetic state with an enhanced electronic specific heat coefficient at $T_C = 74.5 (\pm 0.5)$ K. The ordered magnetic moment of the two nonequivalent uranium ions is 1.12 (1)

and 1.03 (1) μ_B . The thermoelectric power of β -UB₂C is positive and is maximum at 12 K [32].

The connection between boron and carbon atoms results in infinite, one-dimensional zigzag chains, which are isolated from each other and inserted in channels built by metal atoms. These B–C zigzag chains were observed in ordered UBC, ThBC, Th₃B₂C₃, NpBC, and PuBC and in randomly occupied UB_{0.78}C_{1.22} [30]. The carbon atoms in UBC and ThBC occupy the interstices in the UB and ThB sublattice, whereas carbon atoms are considered a stabilizer of actinide borocarbides [33]. The magnetic behavior of UB_{1-x}C_{1+x} (UBC type) in the temperature range from 4.2 to 1000 K was investigated [34]. The UB_{1-x}C_{1+x} alloys had a temperature-independent paramagnetism with typical intermediate valence fluctuation behavior. A short average U–U separation of 3.5 Å was found in UB_{0.78}C_{1.22}, thereby indicating a strong direct U–U 5f overlap.

Compared with its uranium counterpart, ThBC has been sparsely studied by the scientific community, especially its mechanical and thermodynamic properties, which practically hinder its application in the thorium fuel cycle. Therefore, theoretical investigation of these properties would significantly help, especially in the field of nuclear materials, where adequate experimental data are missed. Here, the mechanical and thermodynamic properties of ThBC were investigated by first-principles calculations. Elastic moduli, Poisson's ratio, and the B/G ratio were estimated. Elastic anisotropy was studied on the basis of anisotropic factors and the directional dependence of the bulk modulus and Young's modulus. The ideal tensile and shear strengths of ThBC were obtained by use of strain-stress relationships.

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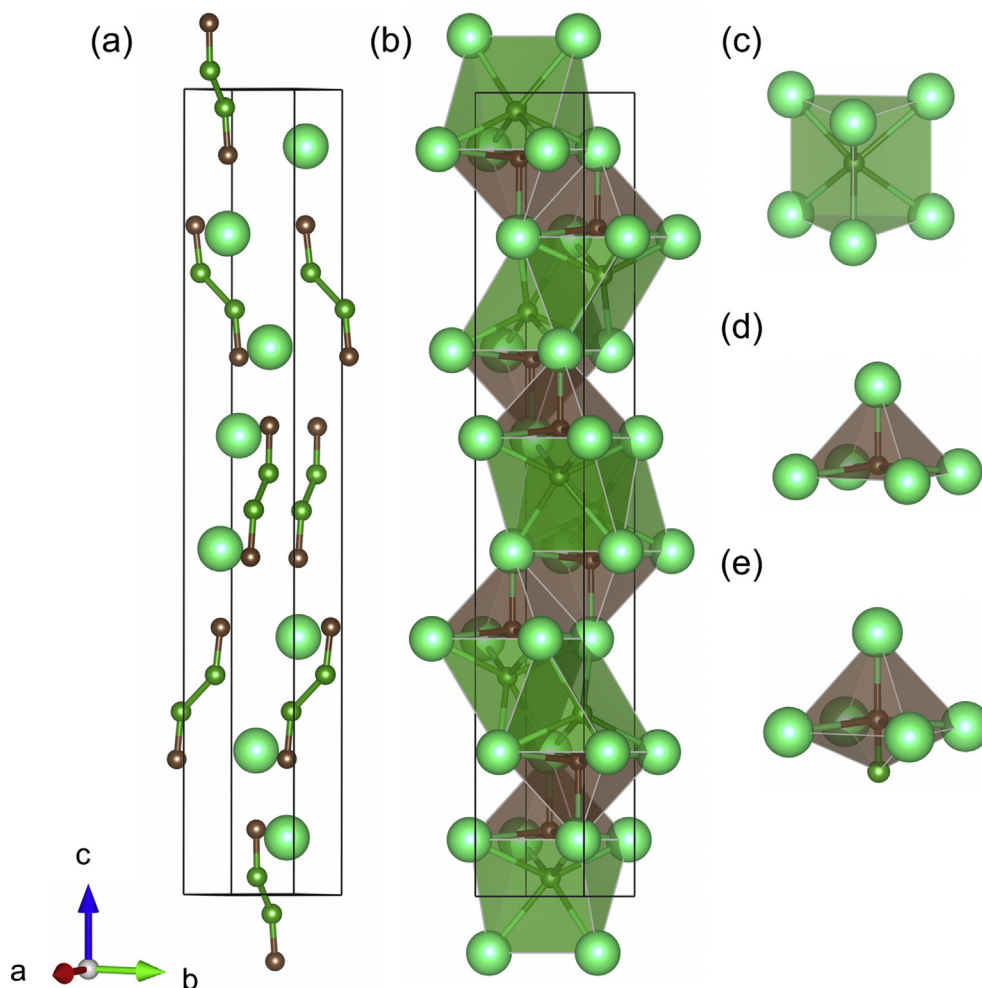


Fig. 1. Crystal structure of ThBC in the view of (a) a zigzag chain and (b) a polyhedron. Building blocks of (c) a B-centered triangular prism, (d) a C-centered square pyramid, and (e) a C-centered octahedron. The large green, small green, and small brown spheres represent the Th, B, and C atoms, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

2. Computational methods

First-principles calculations based on density functional theory were performed within the generalized gradient approximation (GGA) [35] and the local density approximation (LDA) [36]. The projector augmented wave [37] was used as implemented in the Vienna Ab Initio Simulation Package [38]. A cutoff energy of 600 eV for the plane-wave basis and Γ -centered k -point meshes [39] with a separation of $2\pi \times 0.03 \text{ \AA}^{-1}$ were used, which were carefully tested to ensure the convergence of mechanical and thermodynamic properties. The force criterion was set to 0.01 eV/Å when the unit cell and atomic positions were relaxed. Thorium compounds, such as oxides [13], carbides [18], nitrides [28], and hydrides [40], have been investigated with use of the LDA or GGA without a Hubbard U parameter. The GGA and LDA methods can successfully describe the ground-state properties of these thorium compounds, such as structural, elastic, electronic, and thermodynamic properties. Therefore, it is appropriate to use the conventional density functional theory method to investigate the physical and chemical properties of ThBC.

Accurate crystal elastic constants were determined from the strained structures, and the various mechanical moduli were estimated by use of the Voigt-Reuss-Hill approximation [41]. The calculation of ideal strength was first proposed by Roundy et al. [42], and then this method was successfully applied to various systems [43–45]. To determine the ideal tensile strength, the lattice vectors of the unit cell were incrementally deformed along the direction of the applied strain. At each

step, the cell parameters, the cell volume, and the atomic positions were allowed to relax until all the components of the Hellmann-Feynman stress tensors orthogonal to the applied strain were less than 0.05 GPa. The tensile strains were applied along various directions to identify the weakest tensile direction. Once the weakest tensile direction had been obtained, shear strains along various directions in the easy-slip plane were applied to determine the critical shear stress.

Phonon calculations were performed with the PHONOPY code [46–48]. For ThBC, a $3 \times 3 \times 1$ supercell and k -meshes of $2\pi \times 0.04 \text{ \AA}^{-1}$ were chosen. Under the quasi-harmonic approximation [48–50], the contribution of phonons to the Helmholtz free energy is given by

$$F_{ph} = \frac{1}{2} \sum_{q,\nu} \hbar\omega(q, \nu) + k_B T \sum_{q,\nu} \ln \left[1 - \exp\left(-\frac{\hbar\omega(q, \nu)}{k_B T}\right) \right],$$

where $\omega(q, \nu)$ is the phonon frequency at wave vector q and band ν , T is temperature, and k_B and \hbar denote the Boltzmann constant and the reduced Planck constant, respectively. The entropy and heat capacity at constant volume are defined as

$$S = -k_B \sum_{q,\nu} \ln \left[1 - \exp\left(-\frac{\hbar\omega(q, \nu)}{k_B T}\right) \right] - \frac{1}{T} \sum_{q,\nu} \frac{\hbar\omega(q, \nu)}{\exp(\hbar\omega(q, \nu)/k_B T) - 1}$$

and

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