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# Nature of low compressibility and anisotropic elasticity in $YbB_2$

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ABSTRACT

Recent high-resolution synchrotron X-ray diffraction experiments (Kalkan et al., 2012) investigated bulk modulus and compressibility of high purity $YbB_2$ and found that its compressibility can be compared even to that of diamond. In this paper we investigate the structural, compressibility and electronic properties of rare-earth $YbB_2$ using density functional theory to illuminate the nature of its low compressibility and anisotropic elasticity. The calculated results are in agreement with the available theoretical and experimental data and confirm $YbB_2$ as a hard material. The nature of $YbB_2$ hardness and low compressibility is revealed by analyses of its electronic and directional bonding properties: it lies in very strong in-layer and strong enough between-layer bonds. The isotropic bulk modulus, shear modulus, Young's modulus, elastic anisotropy, wave velocities and Debye temperature of $YbB_2$, under ambient and pressures up to 300 GPa are also discussed. Pressure induces expected behavior in most of these properties (monotonic increase), except in elastic constant $c_{44}$, which softens and could lead to elastic instability. Furthermore, anisotropic factors, which are very different at zero pressure, give similar values at the pressure of 300 GPa, closing the gap between compressional and shear anisotropy. Ductility unexpectedly increases with pressure.



## 1. Introduction

The experimental observation of super-hard materials has attracted much interest due to their importance in technology and industrial applications. These materials have excellent mechanical properties such as high hardness, low compressibility, high melting point, high resistance to penetration and low plastic deformation [1–11]. As many of these materials have limited applications (like diamond) or do not occur naturally (making them very expensive), there exists a need to develop new materials comprising the above mentioned properties. One of the families of materials falling into this category are transition metal diborides having their bulk moduli in the range between 300 and 400 GPa [12,13]. Recent theoretical studies proposed and proved rare-earth diboride compounds having the similar properties making them suitable candidates for incompressible and hard materials [14,15].

Elastic properties of $YbB_2$ are important due to fundamental solid-state phenomena such as equation of state, compressibility and anisotropy. Elastic stiffness coefficients are essential for many applications related to mechanical properties of $YbB_2$ such as internal strain, thermo-elastic stress and load deflection. It is also very important to characterize $YbB_2$ crystal under varying pressure upon which elastic stiffness coefficients depend. High pressure study of $YbB_2$ crystals under compression are currently of great interest, due to advances in the generation of ultra-high pressures with diamond anvil cells. High pressure, along with ambient pressure studies on $YbB_2$, can help to understand the mechanism of interaction among the atoms and possible crystal phases of the $YbB_2$-like materials.

Very few efforts have been made to understand the properties of $YbB_2$. Kalkan et al. investigated experimentally $YbB_2$ under high pressure using high-resolution synchrotron X-ray diffraction in a diamond anvil cell and obtained bulk modulus of 182 GPa [16]. The pressure dependent compressibility was also studied up to 20 GPa. Zazoua et al. studied the structures and magnetic phase stability of the rare-earth diboride series of compounds using local density approximation and calculated the mechanical properties, but restricted only to zero pressure and did not discuss the nature of their properties [15]. A description of connection between mechanical and elastic properties of a material was given by Panda and Chandran in their study of elastic constants of $TiB_2$ [17].

This work has three intended aims: first, it will be useful to the first-principles community as well as experimentalists, who are interested in the high pressure physics of structurally and

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experimentally expensive systems, particularly the diboride materials, to gain a better understanding of the kind of information that can reliably be obtained. Second, it is important, from the application point of view, that we model the properties and end up with material based devices. Third, by studying the electronic properties of $YbB_2$ we are able to develop a deeper understanding of its mechanical and elastic properties.

It is well known that the pressure is an important parameter to tune physical properties. Structural parameters and electronic properties of a solid under pressure are closely related to compressibility, hardness, stability and other characteristics, and hence direct information on the characteristics of a crystal can be obtained. Taking into account the so far published findings on physical properties for $YbB_2$, a detail microscopic description of the $YbB_2$ under pressure is essential, because this material provided the recent stimulus for high compressible and super hard materials. In our article we clarify the nature of mechanical and elastic properties of $YbB_2$ by studying its electronic properties and discuss their consequences. This understanding can be further used to model other materials having similar or even better properties.

The rest of the paper is divided in three parts. In Section 2, we have given detailed description of the computational technique we employed for present calculations. The obtained structural parameters, elastic and mechanical properties, electronic densities of states and charge densities at ambient and high pressure properties are discussed in detail in Section 3. Finally in Section 4 important conclusions are presented.

#### 2. Method of computation

In this paper all electronic calculations for $YbB_2$ are performed using plane wave method implemented in ABINIT software package [18], within the framework of density functional theory. The electron–ion interactions are described through the use of Troullier–Martins type pseudopotentials. The generalized gradient approximation (GGA) to the exchange correlation was used for $YbB_2$. A set of convergence tests have been performed on all studied properties in order to correctly choose the mesh of $k$-points and the cut-off kinetic energy plane waves. The energy cut-off of 60 Ha and $12 \times 12 \times 12$ $k$-point mesh ensure that all studied properties differ from the completely converged ones (calculated with cut-off energy of 100 Ha and $k$-point mesh $20 \times 20 \times 20$) by insignificant amounts: pressure by less than 0.1 GPa. elastic constants by less than 1 GPa and electron eigenvalues by less than $10^{-4}$ Ha. The crystal structure and associated equilibrium lattice constant for $YbB_2$ compound have been obtained using the Broyden–Fletcher–Goldfarb–Shanno minimization technique as implemented in ABINIT software package. Elastic constants were calculated using density functional perturbation theory (DFPT) also as implemented in ABINIT software package [19].

## 3. Results and discussion

### 3.1. Structural properties

The structural optimization for minimum total energy condition has been performed to obtain the ground state properties of $YbB_2$. The calculated total energies obtained through optimization process are fitted to third-order Birch–Murnaghan equation of state [20,21]. This yielded the equilibrium total energy and volume, bulk modulus and first order pressure derivative of bulk modulus. Table 1 presents the lattice constants and bulk modulus together with available experimental and theoretical data. The calculated values of lattice constant are in good agreement with available measured and theoretical values, while the bulk modulus agrees very well with other ab initio theoretical value. With respect to the experimental value of bulk modulus, our theoretical value is underestimated, because GGA approximation used in our calculations systematically overestimates the unit cell volume.

**Table 1**
Lattice parameters (in Å) and bulk modulus (in GPa) of $YbB_2$ compared to other theoretical (Ref. [15]) and experimental values (Refs. [16,22]).

| | $a$ | $c$ | $B$ |
|---|---|---|---|
| This work | 3.238 | 3.820 | 145.57 |
| Ref. [15] | 3.159 | 3.838 | 147.68 |
| Ref. [16] | 3.252 | 3.730 | 182.20 |
| Ref. [22] | 3.256 | 3.735 | |

Compressibility is, in general, understood as the extent to which a given solid resists both elasticity and plasticity. To present the compressibility of $YbB_2$, the calculated volume compression as a function of pressure is plotted in Fig. 1. For comparison, the results of $GdB_2$, $LuB_2$ and diamond are also shown in the figure as the representatives of hard and ultra-hard materials. The ultra-incompressibility of $YbB_2$ has been verified by experimental data. As we can see from Fig. 1, density functional calculations slightly overestimate the compressibility of $YbB_2$, which is, again, due to the overestimation of volume by GGA approximation used [23]. By its compressibility $YbB_2$ falls into a group of hard materials comparable to $GdB_2$ and $LuB_2$, but still more compressible than diamond. This is what makes $YbB_2$ a very interesting and useful material.

### 3.2. Elastic properties and the description of hardness

An elastic property of the material reflects the response of the inter-atomic forces between the atoms to an applied stress and is, thus, responsible for many solid state and related thermodynamical phenomenon, such as equation of states, specific heat, Debye temperature, etc. An elastic constant of the material is one of the very crucial tools to determine the relation between strain of the material and applied stress. As $YbB_2$ has a hexagonal unit cell, there are five independent elastic constants, namely $c_{11}, c_{12}, c_{13}, c_{33}$ and $c_{44}$ ($c_{66}$ is equal to $1/2(c_{11} - c_{12})$). Elastic constants at different pressures are given in Fig. 2(a). All constants increase with pressure (up to 300 GPa) as a result of shorter atomic bonds. If compared to only available results (theoretical results by Zazoua et al. [15]), our calculated elastic constants differ by various amounts ranging from 30 to 60 GPa. These differences can be attributed to different methods used, as Zazoua et al. used FP-LAPW method, while we used pseudopotentials to represent the electron–ion interaction and pure plane waves to represent the wave functions. As elastic constants $c_{11}$ and $c_{33}$ regard the resistance in linear compression in $a$- or $c$-direction [24], one can predict that there is a certain measure of elastic anisotropy in $YbB_2$ (for analogy see Fig. 4 showing elastic anisotropy existing inside and between the layers of $YbB_2$). An interesting detail can be mentioned regarding the high pressure behavior of the elastic constants (Table 2). Although the pressure derivatives of all elastic constants at zero pressure are positive, at the pressure of 300 GPa, $dc_{44}/dp$ is negative, indicating that this elastic constant

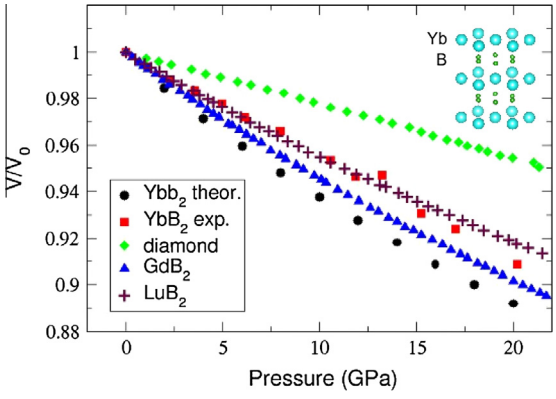


**Fig. 1.** Calculated volume compression of $YbB_2$ compared to other hard and superhard materials (experimental data from Ref. [16]). Inset shows the layered structure of $YbB_2$.