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# Structural and elastic properties of $AlB_2$ compound via first-principles calculations

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**Abstract**

The equilibrium lattice constants, five independent elastic constants and Debye temperature of HCP structure $AlB_2$ are investigated by using a first-principles plane wave method with the relativistic analytic pseudopotential of Hartwigsen, Goedecker and Hutter scheme in the frame of density functional theory. The equilibrium lattice constants obtained are in good agreement with the available experimental data and other theoretical results. No theoretical or experimental data for our calculated elastic constants and Debye temperature are yet available for our comparison.


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*Keywords:* Local density approximation; Elastic constants; Debye temperature; $AlB_2$

## 1. Introduction

The $AlB_2$ structure type and derivatives thereof are among the most frequently occurring ones for intermetallic binary and ternary compounds [1,2]. Transition metal diborides belonging to this family have been studied in some detail because of their potential application in electronic devices to overcome current problems of electromigration, corrosion and diffusion into the semiconductor substrate [3]. Recently, the discovery of superconductivity at $T_c = 39\,K$ in $MgB_2$ [4], which also crystallizes in the $AlB_2$ structure, initiated a strong interest also in s–p diborides. The chemical variability and simplicity of the crystal structure with graphite-like nets of boron atoms separated by aluminum in hexagonal prismatic voids (space group P6/mmm) make this structure type a very interesting one for systematic investigation of crystal chemical and physical properties by experimental as well as theoretical methods, including lattice dynamics properties [5–12], electron–phonon and optical properties [11–16], and high-temperature and high-pressure properties [10].

A first-crystal structure determination by X-ray methods revealed hexagonal symmetry, with complete occupation of both atomic positions according to composition $AlB_2$ [17]. However, density measurements [18,19] indicated defects in the structure. Scarcely described chemical analyses gave different results, e.g., $Al_{1.0}B_2$ [20] or $Al_{0.9}B_2$ [18]. Burkhardt et al. [21] examined the crystal structure and further characterized the phase by $^{11}B$ NMR, electrical resistivity and Hall-coefficient measurements, and discussed the chemical bonding and electronic properties in the light of quantum chemical calculations. Loa et al. [10] studied the crystal structure of $AlB_2$ up to 40 GPa by X-ray powder diffraction. They proposed the compressibility is moderately anisotropic, consistent with the anisotropic bonding properties. In the pressure range they did not observe a

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structural phase transition. Their X-ray diffraction data indicated an Al deficiency of ~11% in agreement with previous reports.

Elastic properties, which are closely related to many fundamental solid-state properties, such as equation of state, specific heat, thermal expansion, Debye temperature, Grüneisen parameter, melting point, and so on, are important in fields ranging from geophysics to materials research, chemistry and physics. The knowledge of elastic constants is essential for many practical applications related to the mechanical properties of a solid: load deflection, thermoelastic stress, internal strain, sound velocities and fracture toughness [22]. From the elastic constants, one can obtain valuable information about the bonding characteristic between adjacent atomic planes and about the anisotropic character of the bonding and about the structural stability of a crystal. Owing to there being few investigations on the elastic properties of $AlB_2$, we here investigate the structures and elastic constants of $AlB_2$ by using a first-principles plane wave method in the frame of local density approximation (LDA). The results obtained are in agreement with the available experimental results and those obtained by other theoretical methods. In Section 2, we briefly review the theoretical methods. The calculated results with some discussion are presented in Section 3.

## 2. Theoretical method

### 2.1. Total energy electronic structure calculations

In this work, we apply a first-principles calculation with a relativistic analytic pseudopotential of Hartwigsen, Goedecker and Hutter (HGH) scheme [23] in the frame of density functional theory (DFT) [24] within LDA. The HGH-type pseudopotential requires about 10 parameters [23]. In our calculations, the kinetic energy cut-off criterion of 10 Hartree is adopted to get the convergence of $10^{-7}$ Hartree in energy. The total energy and the ground-state wave functions are calculated on a $10\times10\times10$ $k$-point mesh. For the exchange–correlation functional, the Perdew-Zunger-Ceperly Alder functional [25] is employed. Applying this method, we have successfully investigated the elastic constants and the thermodynamic properties of $MgB_2$ [26,27] and c-BN [28].

### 2.2. Elastic properties

The elastic constants are defined by means of a Taylor expansion of the total energy, $E(V, \delta)$, for the system with respect to a small strain $\delta$ of the lattice primitive cell volume $V$. The energy of a strained system is expressed as follows [27,29]:

$$E(V,\delta) = E(V_0,0) + V_0\left[\sum_i \tau_i\xi_i\delta_i + \frac{1}{2}\sum_{ij} C_{ij}\delta_i\xi_j\delta_j\right], \quad (1)$$

where $E(V_0, 0)$ is the energy of the unstrained system with equilibrium volume $V_0$, $\tau_i$ is an element in the stress tensor and $\xi_i$ is a factor to take care of Voigt index [29].

There are five independent components of the elastic tensor for $AlB_2$, i.e., $C_{11}$, $C_{12}$, $C_{13}$, $C_{33}$ and $C_{44}$. To obtain all elastic constants for the HCP structure $AlB_2$, we at least need five independent strains listed in Table 1. For each strain, a number of small values of $\delta$ are taken to calculate the total energies for the strained crystal structure $AlB_2$. The calculated $E$–$\delta$ points are then fitted to a second-order polynomial $E(V, \delta)$, and the third-order derivatives of $E(V, \delta)$ with respect to $\delta$ are easily obtained.

### 2.3. Thermodynamic properties

The quasi-harmonic Debye model [30] has been successfully applied to investigate the thermodynamic properties of $MgB_2$ [27] and c-BN [28]. In the quasi-harmonic Debye model, the non-equilibrium Gibbs function $G^*(V; P, T)$ takes the form of

$$G^*(V;P,T) = E(V) + PV + A_{\mathrm{Vib}}(\Theta(V);T), \quad (2)$$

where $\Theta(V)$ is the Debye temperature. The vibrational term $A_{\mathrm{Vib}}$ can be written as [31,32]

$$A_{\mathrm{Vib}}(\Theta;T) = nKT \times\left[\frac{9}{8}\frac{\Theta}{T} + 3\ln(1-\mathrm{e}^{-\Theta/T}) - D(\Theta/T)\right], \quad (3)$$

where $D(\Theta/T)$ represents the Debye integral and $n$ is the number of atoms per formula unit. For an isotropic solid,

Table 1
Strains used to calculate the elastic constants of $AlB_2$ at zero pressure

| Strain ($n$) | Distortion | Energy for distorted system | $\frac{1}{V_0}\frac{\partial^2 E(V,\delta)}{\partial\delta^2}\vert_{\delta=0}$ |
|---|---|---|---|
| 1 | $\varepsilon_{11}=\varepsilon_{22}=\delta$ | $E(V,\delta)=E(V_0,0)+V_0[(\tau_1+\tau_2)\delta+(C_{11}+C_{12})\delta^2]$ | $2(C_{11}+C_{12})$ |
| 2 | $\varepsilon_{13}=\varepsilon_{31}=\delta$ | $E(V,\delta)=E(V_0,0)+V_0[(\tau_5\delta+2C_{44})\delta^2]$ | $4C_{44}$ |
| 3 | $\varepsilon_{33}=\delta$ | $E(V,\delta)=E(V_0,0)+V_0[(\tau_3\delta+1)/C_{33}\delta^2]$ | $C_{33}$ |
| 4 | $\varepsilon_{11}=-\varepsilon_{22}=\delta$ | $E(V,\delta)=E(V_0,0)+V_0[(\tau_1-\tau_2)\delta+(C_{11}-C_{12})\delta^2]$ | $2(C_{11}-C_{12})$ |
| 5 | $\varepsilon_{11}=\varepsilon_{33}=\delta$ | $E(V,\delta)=E(V_0,0)+V_0[(\tau_1+\tau_3)\delta+\frac{1}{2}(C_{11}+2C_{13}+C_{33})\delta^2]$ | $C_{11}+2C_{13}+C_{33}$ |

In the second column, all unlisted elements of strain tensors are set to zero.