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STRUCTURAL AND MECHANICAL PROPERTIES OF ORTHORHOMBIC LiBeH$_3$: AB-INITIO STUDY

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Abstract

The structural parameters and the elastic properties of orthorhombic LiBeH$_3$ material were predicted theoretically using the density functional theory (DFT). The exchange-correlation potential term was treated using the local density approximation (LDA). Our values of the structural parameters and elastic constants predicted for LiBeH$_3$ material agree well with other results of the literature.

The bulk modulus calculated from the BFGS technique is comparable with the value obtained from the elastic constants. The universal anisotropy factor, Young's and shear moduli, Poisson's ratio, Pugh's ratio, Lame's coefficients and the microhardness were also determined for an ideal polycrystalline LiBeH$_3$ material. Based on the results of Poisson's ratio and Pugh's ratio obtained in this work, this hydride material would be classified as a brittle material in nature.

We estimate also the elastic wave velocities, the Debye temperature and the acoustic impedance of the polycrystalline material. Our predicted values obtained from the local density approximation for LiBeH$_3$ material agreed well with the data of the literature obtained from the generalized gradient approximation (GGA).

1. Introduction

Perovskite compounds have attracted much attention of scientists due to their interesting physical and chemical properties and potential broad range of technological applications [1]. As ones of new series of high hydrogen content hydrogen-storage materials, both LiBeH$_3$ and NaBeH$_3$ perovskite-type hydrides have been extensively investigated and comprehensive

experimental and theoretical studies of their properties were the subject of several recent studies [2 – 6]. Using Full Potential-Linearized Augment Plane Wave Method (FP-LAPW+ lo) as implemented in WIEN2k code, Rehmat *et al*. [2] investigated the structural properties, elastic constants and Debye temperature of both cubic and orthorhombic inorganic $LiBeH_3$ and $NaBeH_3$ materials, while the structural phase stability of $NaBeH_3$, $NaMgH_3$ and $Ca(BH_4)_2$ have been investigated by Vajeeston *et al.* [3] using the projector-augmented-wave method. In another work, Vajeeston *et al.* [4] investigated the structural characteristics of $LiBeH_3$, α-$KBeH_3$, $RbBeH_3$ and $CsBeH_3$ ternary materials using the density functional theory (DFT). They found that $LiBeH_3$ compound is one of a promising material for hydrogen storage, because this material has high gravimetric density and can stores up to 15.93% by weight of hydrogen [4].

Using first principle calculations based on DFT with the pseudopotential plane-wave (pp-pw) formalism, Reffas *et al*. [6] studied the structural properties, elastic constants and electronic and optical properties of both cubic $LiBeH_3$ and $NaBeH_3$ perovskites hydrides materials, while Guendouz *et al*. [7] investigated the electronic band structure and optical and thermodynamic properties of $MBeH_3$ (M = Li, Na, and K) ternary hydride materials.

The aim of this work is to study the elastic characteristics of $LiBeH_3$ in orthorhombic phase utilizing first-principle approach. The understanding of the mechanical properties helps in characterizing the material's response to external forces, including its strength, stiffness and deformation behavior. This information is fundamental for assessing the material's suitability for specific applications and helps in optimizing manufacturing and processing techniques.

Our paper is organized as follows: in section 2 we show the computational details based on the first-principles methodology. Section 3 presents some results and their discussion with analysis. Finally, our work is finished with a general conclusion.

2. Method of calculations

The structural parameters and elastic constants of $LiBeH_3$ calculated here were obtained using the CASTEP code [8, 9], which is based on the pp-pw approach in the framework of the DFT.

In this work, we use the local density approximation (LDA) [10] for the description of the exchange-correlation energy term, while for the treatment of the interaction between valence electrons and ions, we employed the Vanderbilt-type ultra-soft pseudo-potentials (USP) [11]. Pseudo-atomic calculations were performed for H-$1s^1$ element, Li-$1s^2 2s^1$ element

and Be-$2s^2$ element, respectively. In order to expand the wave functions, we considered a value of 450 eV for the plane-wave kinetic energy cutoff (E_{cut}), while the Brillouin zone integration of the primitive unit cell was performed according to the Monkhorst-Pack method [12] using 8×6×8 meshes. The equilibrium structural parameters of the crystal were obtained from the geometry optimization using the Broyden-Fletcher-Goldfarb-Shanno (BFGS) minimization scheme [13]. In the geometry optimization procedure, the maximum magnitude of the force on the atom, that on the stress, and as well as on atomic position displacement between computational cycles were maintained below 0.01 eV/Å, 0.02 GPa and 5×10^{-4} Å, respectively. The calculation of total energy was followed by the optimization of the unit cell with self-consistent field tolerance of 5×10^{-6} eV/atom.

3. Results and discussions

3. 1. Structural parameters

Frequently, in the *ab*-initio calculations, the ground state lattice parameters (volume), the bulk modulus and its first order pressure derivative were predicted from the calculated total energy of the system for a primitive unit cell for various values of the lattice constants using the Birch-Murnaghan's equation of state [1, 14]. In our simulation, we have stabilized $LiBeH_3$ as an orthorhombic structure (space group Pnma, No. 62), the conventional unit cell of the orthorhombic $LiBeH_3$ hydride material is shown in Figure 1 [4].

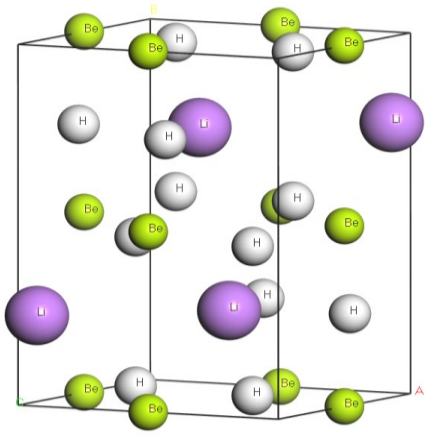


Figure 1. Crystal structure of orthorhombic $LiBeH_3$ hydride material

The theoretically predicted ground state lattice structural parameters (a, b and c) for orthorhombic $LiBeH_3$ material are shown in Table 1. They are compared to available experimental [15] and other theoretical data [2, 4, 5, 7, 16, 17]. Our relaxed structure and the stated experimental structure appear to be in good accord. In this work, the LDA

underestimates the variations from the experimental unit cell parameters by 3.04 % for *a*, less than 0.5 % for *b*, and by 2.74 % for *c*, respectively [15]. These findings demonstrate the validity of the methodology employed in this study, allowing for the use of the optimized lattice constants in further parameter computations such as elastic constants.

Table 1. Optimized equilibrium structural parameters of orthorhombic $LiBeH_3$ material as obtained from LDA, compared to available experimental [15] and other theoretical data [2, 4, 5, 7, 16, 17]

Ref.		This work	[2]	[4]	[5]	[7]	[7]	[15]	[16]	[17]
Exchange-correlation		LDA	GGA PBE	GGA	GGA PBE	GGA	LDA	Exp	-	GGA
Unit cell parameters (Å)	a =	4.498	4.526	4.5361	4.523	4.5232	4.4595	4.639	4.517	3.385
	b =	6.189	6.293	6.2992	6.290	6.3207	6.4595	6.217	6.273	4.703
	c =	4.303	4.404	4.4104	4.401	4.4205	4.4242	4.424	4.387	3.268

3. 2. Elastic properties

It is well known that several solid-state parameters are intimately related to elastic constants. Furthermore, the elastic constants are frequently used to derive various mechanical and thermodynamic properties, such as ductility, hardness, fracture toughness and Debye temperature [14, 18]. It is well known that first principle studies based on DFT are used to obtain reliable results regarding the elastic properties of inorganic compounds [2]. The number of elastic constants is reduced based on the crystal symmetry. In the case of orthorhombic system, there are only nine independent elastic constants, i.e., C_{11}, C_{22}, C_{33}, C_{44}, C_{55}, C_{66}, C_{12}, C_{13}, and C_{23}. The well-known Born stability needs must be satisfied by C_{ij} for an orthorhombic structure [19]:

$C_{ij} > 0$, $(C_{11} + C_{33} - 2C_{23}) > 0$, $(C_{11} + C_{33} - 2C_{13}) > 0$, $[C_{11} + C_{22} + C_{33} + 2 (C_{12} + C_{13} + C_{23})] > 0$, and

$$(C_{11} + C_{22} - 2C_{12}) > 0 \quad (1)$$

The orthorhombic $LiBeH_3$ elastic constants satisfy the Born stability conditions provided by Equation (1). The orthorhombic $LiaBeH_3$ is therefore mechanically stable at atmospheric pressure. Table 2 lists and compares the obtained elastic constants C_{ij} of orthorhombic $LiaBeH_3$

with other theoretical values [2]. Unfortunately, no experimental or other theoretical results for the elastic constants C_{ij} are available in the literature for the orthorhombic $LiaBeH_3$ material.

Table 2. Elastic constants (in GPa) of orthorhombic $LiBeH_3$, in comparison with data of Ref [2]

Elastic constant	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}
This work (LDA)	129.3	130.3	125.6	59.3	47.6	70.2	37.1	33.0	36.3
Ref. [2] (GGA-PBE)	144.9	129.2	143.7	64.7	44.4	68.9	35.6	17.2	38.0

3. 3. Polycrystalline elastic moduli

The elastic constants C_{ij} cannot be measured in the absence of single crystal samples. Instead, it is possible to determine the polycrystalline bulk modulus B and shear modulus G [20-22]. Two main approximations are often employed for such calculations, namely the Voigt (V) and Reuss (R) schemes [23, 24]. In Voigt's approximation, the bulk (B_V) and shear (G_V) moduli of the orthorhombic structure can be presented as follows [25]:

$$B_v = (1/9)(C_{11} + 2C_{12} + 2C_{13} + C_{22} + 2C_{23} + C_{33}) \quad (2)$$

$$G_v = (1/15)(C_{11} - C_{12} - C_{13} + C_{22} - C_{23} + C_{33} + 3C_{44} + 3C_{55} + 3C_{66}) \quad (3)$$

Both moduli, B_R and G_R can be represented as follows using the approximation of Reuss [2]:

$$B_R = 1/[S_{11} + S_{22} + S_{33} + 2(S_{12} + S_{13} + S_{23})] \quad (4)$$

$$G_R = 15/[4(S_{11} + S_{22} + S_{33}) - 4(S_{12} + S_{13} + S_{23}) + 3(S_{44} + S_{55} + S_{66})] \quad (5)$$

where the elastic compliance constants S_{ij} are listed in Table 3.

Table 3. Elastic compliance constants (in 10^{-2} GPa) of $LiBeH_3$ material in the orthorhombic phase, in comparison with data of Ref [2]

Elastic constant	S_{11}	S_{22}	S_{33}	S_{44}	S_{55}	S_{66}	S_{12}	S_{13}	S_{23}
This work (LDA)	0.87	0.88	0.90	1.69	2.10	1.42	- 0.20	- 0.17	- 0.20
Ref. [2] (GGA-PBE)	0.74	0.88	0.75	1.54	2.24	1.45	- 0.19	- 0.03	- 0.21

Using the Hill model, both the bulk modulus and the shear modulus are the arithmetic averages of Voigt (V) and Reuss (R) bounds [25], they are expressed as follows:

$$B = \left(B_V + B_R\right)/2 \text{ and } G = \left(G_V + G_R\right)/2 \quad (6)$$

To provide an accurate measure of the elastic anisotropy, the universal anisotropy factor (A^U) was often used. Since A^U may apply to all the crystal symmetries, it is referred to as universal anisotropy factor [23], it can be written as [23]:

$$A^U = 5\left(G_V / G_R\right) + \left(B_V / B_R\right) - 6 \geq 0 \quad (7)$$

For elastic isotropic material, A^U is zero [23], while any departure from zero corresponds to the degree of elastic anisotropy. The value (~ 0.14) of A^U indicates a weak degree of elastic anisotropy for the orthorhombic $LiBeH_3$ compound, compared to $CeCoO_3$ material ($A^U = 0.532$) [23].

The rigidity of materials is affirmed after calculate Young's modulus (E) [26]. Young's modulus (E) and Poisson's ratio (v) may be calculated using the Hill approximations of the bulk (B) and shear (G) moduli as follows: $E = 9BG/\left(3B + G\right)$ and $\upsilon = \left(3B - 2G\right)/2\left(3B + G\right)$ [27]. The rigidity of the material can be also checked by calculating the microhardness parameter H. Several expressions were used to calculate the microhardness of materials [28, 29]; one of these expressions is defined as: $H = E\left(1 - 2\upsilon\right)/6\left(1 + \upsilon\right)$ [30]. The orthorhombic $LiBeH_3$ structure's predicted bulk, shear, and Young's moduli, as well as Poisson's ratio are listed in Table 4 for the Voigt, Reuss, and Hill approaches, along the theoretical results of Rehmat *et al* [2]. From the Table 4, we can note that our value (66.43 GPa) of the aggregate bulk modulus calculated from the elastic constants agrees well with our data (69.47 GPa) obtained from the BFGS technique. Furthermore, our resulted bulk moduli and those determined by Rehmat *et al* [2] have good agreement. To the best of authors' knowledge, there are no experimental data reported in the literature to make more comparison.

The mechanical behavior (ductile/brittle behavior) of a material can be often predicted according to Pugh's ratio (B/G) [31]. A material is ductile if the B/G ratio is greater than 1.75, while if B/G ratio is lower than 1.75, it is classified as brittle material [32, 33]. At zero-pressure, the value 1.25 of the B/G ratio for the orthorhombic $LiBeH_3$ is less than 1.75. Therefore, this compound can be classified as brittle material.

Table 4. Calculated bulk moduli B, B_v and B_R (GPa), shear moduli G, G_v and G_R (GPa), Young's modulus E (GPa), micro-hardness H (GPa), B/G ratio, and Poisson's ratio v for orthorhombic $LiBeH_3$ along the theoretical results of Rehmat et al [2].

Parameter	B_V	B_R	B	G_V	G_R	G	E	H	B/G	ν
This work (LDA)	66.45	66.41	66.43	54.01	52.53	53.27	126.1	11.24	1.25	0.18
Ref. [2] (GGA-PBE)	66.65	66.64	66.64	57.41	55.42	56.42	132	12.45	1.18	0.17

The Poisson's ratio *v* measures the stability of the crystal against shearing, formally takes values between -1 and 0.5 [2]. For systems with a mainly central interatomic interaction (i.e. ionic crystals), the value of *v* is usually close to 0.25 [34]. For covalent materials *v* is small (*v* = 0.1), while for metallic materials *v* = 0.33 [2]. For the orthorhombic $LiBeH_3$ material, the Poisson ratio *v* is less than 0.25 which indicates that the chemical bonds in this material are characterized by an ionic-covalent mixture [2].

For isotropic solid, the Lame's first parameter λ is frequently obtained from the Young's modulus *E* and the Poisson's ratio *v* as follows: $\lambda = vE/[(1+v)(1-2v)]$ [35]. The value of λ for the isotropic $LiBeH_3$ material is 30.92 GPa, it is very lower than that (94.51 GPa) of cubic perovskite $BaHfO_3$ material [35].

3. 4. Elastic wave speed and Debye temperature

Thermal properties of materials are the basis of solid-state physics and technological applications [36, 37]. The Debye temperature θ_D of material is one among important thermo-dynamic parameters, which must determined precisely, this because θ_D is related to many other physical properties of solid, especially the elastic constants, the specific heat, the acoustic wave speed, the thermal conductivity and the melting temperature [38-40]. Frequently the Debye temperature θ_D was calculated from mean acoustic wave speed v_m as follows [41]:

$$\theta_D = \frac{\hbar}{k_B}\left[\left(6\pi^2 n \frac{N_A \rho}{M}\right)\right]^{1/3} v_m \qquad (8)$$

where, $\hbar = h/2\pi$, h indicates the Planck's constant, N_A indicates the Avogadro's number, ρ indicates the mass density of the crystal or the substance, M indicates the molecular weight, k_B indicates the constant of Boltzmann and n is the number of atoms constituted the molecule.

The mean value of the acoustic wave speed v_m for aggregate polycrystalline solids can be determined as follows [42-44]:

$$v_m = \left[\frac{1}{3} \left(\frac{2}{{v_t}^3} + \frac{1}{{v_l}^3} \right) \right]^{-1/3} \tag{9}$$

where v_l and v_t indicate the longitudinal and transverse elastic wave speeds, respectively.

The longitudinal elastic wave speed v_l and the transverse elastic wave speed v_t can be determined from the elastic moduli as follows [42-44]:

$$v_l = \left(\frac{3B + 4G}{3\rho} \right)^{1/2}, \text{ and } v_t = \left(\frac{G}{\rho} \right)^{1/2} \tag{10}$$

where ρ is the gravimetric density, B is the bulk modulus and G is the shear modulus.

The mass density of the substance called also the gravimetric density is the ratio of the mass to the volume; it is expressed in kg/m^3 or in g/cm^3. It is given as follows: $\rho = MZ / N_A V$ [45-47], where M is the molecular weight, which is expressed in 10^{-3} kg, Z is the number of molecules per unit cell, V is the unit cell volume, which is expressed in m^3, and N_A is the Avogadro's number.

Our obtained values of the longitudinal, transverse and mean acoustic wave speeds and Debye temperature θ_D of $LiBeH_3$ material in orthorhombic phase are narrated in Table 5. To achieve some comparability with other works, our results are compared with these reported in Ref. [2].

Therefore, we predicted the acoustic behavior of $LiBeH_3$ by computing the so-called acoustic impedance Z. This later may be calculated using the following expression: $Z = (\rho G)^{1/2}$ [48], where G denotes the shear modulus while ρ is the gravimetric density. The acoustic impedance Z of $LiBeH_3$ material has been found at around 7.49×10^6 Rayl, it is lower than the values 19.24×10^6 Rayl and 17.88×10^6 Rayl reported for Ti_2GaB and Zr_2GaB materials, respectively [48].

We can observe from Table 5 that our predicted values of all the mass density, the elastic wave speeds and the Debye temperature θ_D of $LiBeH_3$ material are in good agreement in comparison to the results reported the Ref [2]. The deviation between the value (1286 K) of θ_D predicted here and the theoretical data (1330.5 K) reported by Rehmat *et al* [2] is less than 3.35%. As far as we know, there is no data available in literature on the acoustic impedance for the $LiBeH_3$ material to make comparison.

Table 5. Gravimetric density ρ, longitudinal v_l, transverse v_t and average v_m sound speeds, and Debye temperature θ_D of the orthorhombic $LiBeH_3$ material, in comparison with data of Ref [2]

Parameter	ρ (g/cm^3)	v_l (km/s)	v_t (km/s)	v_m (km/s)	θ_D (K)	Z (Rayl)
This work (LDA)	1.052	11.431	7.116	7.842	1286	7.49×10^6
Ref. [2] (GGA-PBE)	1.00	11.862	7.480	8.232	1330.5	-

4. Conclusion

In this study, orthorhombic $LiBeH_3$'s structural characteristics and elastic constants were estimated using the DFT. We found that the values of the lattice parameters determined in this work are in agreement with the experimental ones that have already been published in the literature. It is discovered that the orthorhombic $LiBeH_3$ is mechanically stable. Additionally, for this hydride, we computed the ideal polycrystalline bulk modulus, shear modulus, Young's modulus, Poisson's ratio, Lame's coefficients and microhardness. This hydride has a B/G ratio that is less than 1.75. It can thus be categorized as fragile material. We also predicted the universal anisotropy factor, the elastic wave velocities, the Debye temperature and the acoustic impedance of our material of interest. Our obtained values are in good agreement with other data of the literature.

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