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Electronic, phonon and superconducting properties of LaPtBi half-Heusler compound

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ABSTRACT

In the framework of density functional theory based on plane wave pseudopotential method and linear response technique, we have studied the electronic, phonon and superconducting properties of LaPtBi half-Heusler compound. The electronic band structure and density of states show that it is gapless semiconductor which is consistent with previous results. The positive phonon frequencies confirm the stability of this compound in cubic MgAgAs phase. Superconductivity is studied in terms of Eliashberg spectral function ($\alpha^2F(\omega)$), electron-phonon coupling constants (λ). The value of electron-phonon coupling parameter is found to be 0.41 and the superconducting transition temperature is calculated to be 0.76 K, in excellent agreement with the experimentally reported values.

1. Introduction

Topological insulators (TIs) are one of the most prominent class of materials in condensed matter physics and material science due to their valuable scientific significant and broad potentials applications [1–4]. TIs show non-trivial topology in the band structure because they have insulating features in the interior while metallicity at the surface [2–5]. HgTe semi-metal is the first predicted and realized two-dimensional topological insulator (2DTIs) [6,7]. Thereafter several other families of materials for three dimensional topological insulators (3DTIs) have been proposed theoretically and experimentally [8]. The half-Heusler intermetallic compounds are the dominant class predicted as topological properties. They crystallize in MgAgAs-type cubic structure with the F-43 m space group having the composition XYZ, where X is rare-earth or transition metal, Y is transition metal and Z is a p-block element [9]. The XYZ cubic structure can be understood by the filling of 'X' atom into a YZ zinc blende structure. Besides the existence of topological insulators, the half-Heusler compounds also exhibit non-centrosymmetric superconductivity [10,11]. The discovery of superconductivity in half-Heusler compounds with MgAgAs-type structure has drawn great interest to explore the superconductivity in other systems with similar structure. Interestingly some of the Platinum-bismuthides e.g. LuPtBi, YPtBi and Palladium-bismuthides e.g. ErPdBi, CePdBi, LuPdBi are found to exhibit band inversion which makes them promising candidates for topological superconductivity [12–19]. Very recently Shrivastava et al. [20] have studied superconducting properties of LuPtBi in terms of electron-phonon interaction theoretically using density functional linear response theory.

In the present paper, we have investigated the electronic, phonon and superconducting properties of LaPtBi half-Heusler compound in its MgAgAs cubic structure using plane wave pseudopotential method with generalized gradient approximation (GGA). Various studies have been done on the electronic structure of LaPtBi HH compound [10,21–25] so far, therefore in the present paper, we briefly describe the electronic properties along with the linear response approach for lattice dynamics and electron-phonon interactions. The Eliashberg spectral function ($\alpha^2F(\omega)$) and electron-phonon coupling constant (λ) are calculated and compared with the corresponding phonon density of states in detail. Using the calculated value of λ, the superconducting transition temperature (T_C) is evaluated and compared with experimental results [10,19].

2. Computational method

All the calculations reported in this paper have been performed using density functional theory (DFT) [26]. For electronic structure and associated properties of LaPtBi, we have used the full-potential linearized augmented plane wave (FP-LAPW) method [27] with generalized gradient approximation (GGA) scheme of Perdew, Burke and Ernzerhof

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(PBE) [28] for exchange and correlation effects with non spin polarized calculations. The energy convergence is achieved by expanding the basis function up to $R_{MT} * K_{max} = 7$, where R_{MT} is the smallest atomic radius in the unit cell and K_{max} refers to the magnitude of the largest k vector in the plane wave expansion. The maximum value for partial waves inside the atomic sphere is $l_{max} = 10$, while the charge density is Fourier expanded up to $G_{max} = 12$ (a.u.)$^{-1}$. Self-consistent calculations are converged when the total energy of the system is stable within 10^{-4} Ry. Monkhorst-Pack [29] **k**-points grid of $10 \times 10 \times 10$ is used to sample the Brillouin zone for electronic structure calculations. Phonon dispersion curves, phonon density of states in the cubic phase of LaPtBi are calculated using the plane wave pseudopotential method as implemented in QUANTUM ESPRESSO code [30] with density functional perturbation theory (DFPT) [31]. We have used the norm-conserving pseudopotential for describing the interaction between the valence electrons, nuclei and the core electrons [32,33]. The convergence is achieved with a kinetic energy cut-off 150 Ry. which is sufficient to fully converge all properties. The force constants for phonon dispersion calculations are obtained using $5 \times 5 \times 5$ **q**-mesh in the first Brillouin zone.

3. Results and discussion

LaPtBi crystallizes in the MgAgAs-type fcc cubic structure with space group F-43 m (no.216), where La, Pt and Bi atoms are located at 4b (0.5,0.5,0.5), 4c (0.25,0.25,0.25) and 4a (0,0,0) Wyckoff positions respectively. The crystal structure of it shown in Fig. 1 (inset), in which it consists of three interpenetrating, face-centered-cubic lattices with Pt sitting at the unique site. It can be easily understood by the filling of La atoms into a PtBi zinc blende structure. For the calculations of the ground state properties such as the equilibrium lattice constant (a_0), bulk modulus (B), and its pressure derivative (B′), we have calculated total energy as a function of unit cell volume and fitted to Birch-Murnaghan's equation of state [34] and is displayed in Fig. 1. The calculated values of a_0, B and B′ are presented in Table 1 together with available experimental and theoretical [10,21,24,25,35,36] results which show very good agreement.

With the optimized lattice constant of LaPtBi, we have calculated the electronic band structure (BS) along the high symmetry direction of the Brillouin zone and presented in Fig. 2(a). The Fermi level is fixed at origin. The total and partial density of states at ambient pressure are shown in Fig. 2(b). Various studies on the electronic structure of LaPtBi have been done so far which reveal that it is topologically nontrivial and show semi metallic as well as gapless semiconductor nature [10,21–25]. Our present study also shows that LaPtBi is gapless semiconductor i.e. the band gap is closed through touching of the valence and conduction bands at the Fermi level E_F because it contains heavy metals such as La, Pt and Bi and is consistent with previous results [10,21]. From Fig. 2(a), it can be noticed that the bands below the Fermi level are mainly due to the 'p' state of Bi and 'd' state of Pt atoms (Fig. 2(b)). The band structure near the Fermi level at the Γ point is determined mainly by PtBi with the zinc blende structure, and the 'd' and 'f' states of La participate in the band structure additively.

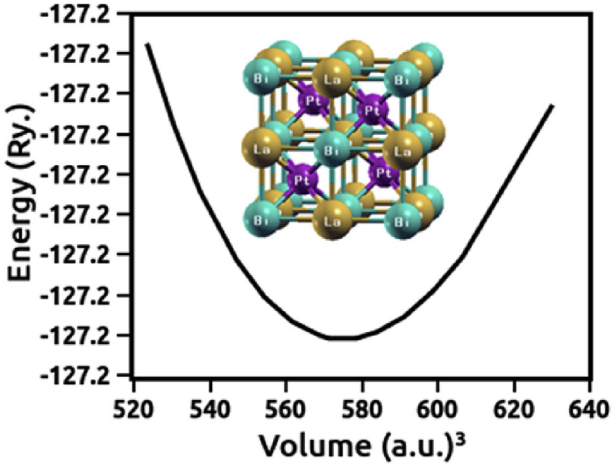

Fig. 1. Variation of total energy with unit cell volume and inset crystal structure of LaPtBi half-Heusler compound in cubic (MgAgAs-type) phase.

Table 1
Calculated lattice parameter (a_0), bulk modulus (B), pressure derivative of bulk modulus (B') and superconducting transition temperature (T_C) of LaPtBi half-Heusler compound in cubic (MgAgAs-type) phase. T_C is compared with other ternary Bi based HH compounds.

Solid	a_0 (Å)	B (GPa)	B′	T_C (K)
LaPtBi				
Pre. (Full-potential)	6.9606	78.91	4.73	–
(Pseudopotential)	6.985	79.6	4.51	0.76
Exp.	6.83[a], 6.8529[b], 6.867[c], 6.829[d]	–	–	0.9[g], 0.7[b]
Theo.	6.90[e], 6.82[f]	–	–	–
LuPtBi				1.1[h],1.0[i]
YPtBi				0.77[j]

[a] Ref. [35].
[b] Ref. [10].
[c] Ref. [21].
[d] Ref. [36].
[e] Ref. [24].
[f] Ref. [25].
[g] [19].
[h] [20].
[i] [12].
[j] [13].

The phonon dispersion curves (PDC) of LaPtBi along high-symmetry directions in the Brillouin zone are shown in Fig. 3(a) which reveal that, all the phonon modes have positive frequencies, and there are no phonon branches which show negative frequency. This picture ensures that the LaPtBi half-Heusler is dynamically stable in cubic MgAgAs-type phase. Nine vibrational modes appear due to the presence of three atoms in the primitive unit cell of LaPtBi. Out of them, the first three are acoustic and rest are the optical modes. The phonon dispersion curves can be separated into two apparent regions: a low-frequency band (LFB) region from 0 to 97 cm^{-1} and a high-frequency band (HFB) region from 115 to 143 cm^{-1}. A narrow gap of about 18 cm^{-1} between these regions comes from the mass difference between the different types of atoms in the unit cell. The LFB is formed by the three acoustic and three optical branches, while the HFB contains the remaining three optical phonon branches. In the PDC, the transverse optical (TO) and longitudinal optical (LO) branches are splitted but are degenerate (around 125 cm^{-1}) at the zone centre Γ point. Fig. 3(a), reveals that, the acoustic and optical branches do not overlap but the band gap between them is very small. The calculated PDC for LaPtBi agree well with Ref. [25]. Fig. 3(b) shows the total and partial phonon density of states of LaPtBi which shows that, the phonon state in the acoustic region is mainly contributed by the vibration of Pt atom with considerable contribution of Bi atom. La and Bi atoms show the most contribution in the highest optical phonon branches. We have presented the frequency-dependent Eliashberg spectral function $\alpha^2F(\omega)$ in Fig. 4. The features of this function are very analogous to that of phonon density of states. A comparison of the Eliashberg spectral function with the phonon density of states explains that the phonon modes in the entire frequency range contribute to the electron-phonon interaction. It is seen from Fig. 4, that there is one highest peak which is similar with phonon density of states. By employing the linear response method and Migdal-Elishberg theory [37,38], the integration of the Eliashberg spectral function gives the average electron–phonon coupling constant (λ), which represents a good measure of the overall strength of the electron–phonon interaction and it is given by