THE STRUCTURAL, ELASTIC, ELECTRONIC AND OPTICAL PROPERTIES OF LaPdBi COMPOUND

N. KOROZLU*
Department of Physics, Faculty of Art and Science, Erzincan University, Basbaglar, Erzincan, TURKEY.

K. COLAKOGLU
Department of Physics, Faculty of Art and Science, Gazi University, Teknikokullar, Ankara, TURKEY.

E. DELIGOZ
Department of Physics, Faculty of Art and Science, Aksaray University, Aksaray, TURKEY.

G. SURUCU
Department of Physics, Faculty of Art and Science, Gazi University, Teknikokullar, Ankara, TURKEY.

Abstract. - We have studied the LaPdBi compound without spin polarization by performing ab initio calculations within the GGA approximations. The some basic ground state physical properties, such as lattice constant, bulk modulus, second-order elastic constants ($C_{ij}$), the electronic band structures, and some optical parameters are calculated, and compared with the available experimental and theoretical data.

Keywords
Ab-initio, Optical properties, Elastic properties, Band Gap energy

The search for advanced thermoelectric materials continues to shift from binary to ternary and higher order compounds [1]. MNiSn (M=Ti, Zr, Hf) compounds which are crystallized in the MgAgAs structure and which are characterized by the existence
of a gap or pseudo-gap in the Fermi level [2]. This behaviour makes these compounds attractive candidates for a study of thermoelectric properties. LaPdBi compound is this-type of material and Cook et al. have reported that LaPdBi and GdPdBi may be attractive candidates for thermoelectric cooling applications [1].

However, LaPdBi compound is thermoelectric material, also known as ternary half-Heusler compounds [3], Yang et al [4] have studied crystal structures and electronic properties of these material families and explained some properties of LaPdBi. Haase et al [5] have reported structural properties of LaPdBi. In present work, the structural, elastic, electronic and optical properties of LaPdBi are investigated using density functional theory, in detail. The calculated results are demonstrated in available format by comparing with theoretical and experimental data.

We have performed the plane-wave pseudopotential approach to the density functional theory (DFT) by Cambridge Sequential Total Energy Package (CASTEP) code [6]. The electronic wave functions were obtained by using a density-mixing minimization method for the self consistent field (SCF) calculation, and the structures were relaxed by using the Broyden, Fletcher, Goldfarb and Shannon (BFGS) method [7]. It solves the quantum mechanical equation for the electrons within the density functional approach in the generalized gradient approximation (GGA). For GGA, the exchange-correlation functional of Perdew-Burke-Ernzerhof was used [8]. The tolerances for geometry optimization were set as the difference in total energy being within \(5 \times 10^{-6}\) eV/atom, the maximum ionic Hellmann-Feynman force within 0.01 eV/Å, the maximum ionic displacement within \(5 \times 10^{-4}\) Å, and the maximum stress within 0.02 GPa. The interactions between electrons and core ions are simulated with ultrasoft Vanderbilt pseudopotentials [9]. The wave functions are expanded in the plane waves up to a kinetic-energy cutoff of 600 eV. The numerical integration of Brillouin zone was performed using an \(8 \times 8 \times 8\) Monkhorst-Pack k-point sampling procedure for this compound.

First of all, the equilibrium lattice parameter has been optimized and calculated value is given in Table 1 with the experimental and theoretical data [4-5]. The cell volume, bulk modulus and band gap energy have also been calculated and listed in Table 1. The calculated lattice parameter agrees well with experimental and theoretical data.

The present first-principles code (CASTEP) has the band structures and density of states (DOS) for LaPdBi. The obtained results for high symmetry directions are shown in Fig. 1. The position of the Fermi level is at 0 eV. The total electronic (DOS) corresponding to the present band structures are, also, depicted in Fig.1. This compound has an indirect band gap along the X direction and the obtained band gap is listed in Table 1 together with the other theoretical data [4].

The elastic constants are important physical properties of a solid and their precise
Table 1: Calculated equilibrium lattice constants ($a_0$), cell volume ($V$), bulk modulus (B) and band gap energy ($E_g$) with available experimental and theoretical data for LaPdBi in MgAgAs structure.

<table>
<thead>
<tr>
<th>Material</th>
<th>Structure Type</th>
<th>References</th>
<th>$a_0$ (Å)</th>
<th>B (GPa)</th>
<th>V (Å³)</th>
<th>$E_g$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LaPdBi</td>
<td>MgAgAs</td>
<td>Theoretical $^a$</td>
<td>6.825</td>
<td>....</td>
<td>....</td>
<td>0.31</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Experimental $^b$</td>
<td>6.825</td>
<td>....</td>
<td>317.90</td>
<td>....</td>
</tr>
</tbody>
</table>

$^a$REF.4
$^b$REF.5

Figure 1: Calculated band structure and DOS of LaPdBi in MgAgAs phase.

evaluation provides valuable information on the mechanical behaviour of any material. Here, to calculate the elastic constants ($C_{ij}$), we have used the “stress-strain” technique [10, 11], and the calculated results for LaPdBi are given in Table 2. We cannot make any comparisons for elastic constants of LaPdBi because there are not available experimental and theoretical data in the literature.

The traditional mechanical stability conditions on the elastic constants for cubic structure [12] are given to be $C_{11}>0$, $C_{44}>0$, $C_{11}>|C_{12}|$, $|C_{11}+2C_{12}|>0$. Our elastic

Table 2: The calculated elastic constants (in GPa) for LaPdBi

<table>
<thead>
<tr>
<th>Material</th>
<th>Reference</th>
<th>$C_{11}$</th>
<th>$C_{12}$</th>
<th>$C_{44}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>LaPdBi</td>
<td>Present</td>
<td>135.75</td>
<td>78.42</td>
<td>30.49</td>
</tr>
</tbody>
</table>
constants listed in Table 2 obey these stability conditions.

Some optical properties of LaPdBi have been computed based on traditional Kramers-Kronig transformation [13]. The real and imaginary parts of dielectric function on the range of 0–30 eV for LaPdBi are displayed in Fig. 2. The main peaks of the real part for LaPdBi occur at 1.15 eV. An important characteristic of $\epsilon_1(\omega)$ is the zero frequency limit $\epsilon_1(0)$, which is the electronic part of the static dielectric constant. For LaPdBi, static dielectric constant $\epsilon_1(0)$ is found to be 23.0. For the imaginary part of the dielectric function for the LaPdBi, the absorption starts at about 0.23 eV. These points are $\Gamma_v$-$X_c$ splitting, which gives the threshold for direct optical transitions between the absolute valence band maximum and the first conduction band minimum. This is known as the fundamental absorption edge [14].

![Dielectric function](image)

**Figure 2**: The real (black line) and imaginary (red line) part of dielectric function for LaPdBi as a function of photon energy.

The dispersion curves ($n(\omega)$) for LaPdBi are plotted in Fig. 3, and the value of refractive index $n(0)$ is found as 4.81. From Fig. 3, we have calculated the extinction coefficients ($k(\omega)$) to be 0.36 of LaPdBi.

Finally, from the real and imaginary parts of the complex dielectric response function, the electron energy-loss function can easily be obtained. It is the imaginary part of the reciprocal of the complex dielectric function, and its main peak is called
Figure 3: Refractive index $n$ (black line) and extinction coefficient $k$ (red line).

Figure 4: Loss function.
Plasmon frequency. Our result is displayed in Fig. 4. The energy loss spectra do not show any distinct maxima in the range of about 0–10 eV. We have calculated the Plasmon frequency to be 15.12.

CONCLUSION

The first-principles pseudopotential calculations have been performed on the LaPdBi compound. Our present key results are on the structural, elastic, electronic and optical properties for LaPdBi. The lattice parameters are excellent agreement with the experimental and theoretical values. The computed band structure shows that LaPdBi is a semiconductor with energy gap of 0.23 eV. We hope some of our results, such as optical properties estimated for the first time in this work, will be tested experimentally and theoretically in future.

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REFERENCES