Refractive index of AlAs and AlSb compounds: An *ab-initio* study

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Refractive index of AlAs and AlSb compounds: An ab-initio study

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Abstract

Using the Full Potential Linear Muffin Tin Orbital (FP-LMTO) method, we have explored the electronic and optical properties as well as refractive index of zinc blende type AlAs and AlSb compounds. The ground-state properties such as lattice constants, bulk modulus and its pressure derivatives are calculated and compared with available results. The optical properties including the dielectric function, electron energy-loss spectrum and refractive index are calculated and also analyzed.

Keywords: Ab-initio study, Total Energy Calculations, Optical properties, Refractive index

1. Introduction

The group III-V zinc blende type binary compounds have attracted much attention for their potential application in electronic industry. In the recent past decades, number of experimental and theoretical [1-3] investigations were carried out on electronic, optical, mechanical and thermodynamic properties of these compounds. AlAs and AlSb semiconductors belong to this group. These materials are one of the important electronic and optical materials and they are used in the field of electronic device fabrication [4, 5]. In the present work we have investigated the electronic and optical properties as well as refractive index of titled compounds using the FP–LMTO method within generalized gradient approximation.

2. Crystal structure and Methodology

At ambient conditions, AlAs and AlSb compounds crystallizes in zinc blende type structure with the space group F4-3m (No. 216) [6]. The unit cell contains 4 cation (Al) and 4 anion (As/Sb) atoms. The position of Al atom is (0, 0, 0) and As/Sb atom is at (0.25, 0.25, 0.25). The schematic crystal structure diagram of these compounds is shown in Figure 1.

All the calculations were done based on the density functional theory. We employed the full potential linear muffin-tin orbital (FP-LMTO) method implemented in the LmtART package [7]. The generalized gradient approximation was used as the exchange-correlation potential in the perdeuw 96 approach [8]. Brillouin zone integrations were performed by using (8×8×8) tetrahedron special point grids [9]. The scalar semi-relativistic effects were taken into account.
3. Results and discussion

3.1 Total Energy and their related properties

The electronic band structure calculation has been carried out for the titled compounds in zinc blend structure. The total energy as a function of cell volume is calculated for these compounds in a manner similar to our earlier work [10]. The calculated total energy versus cell volume is shown in Figure 2. The equilibrium lattice constant, bulk modulus and its pressure derivatives of these compounds were estimated by fitting the total energies to the Birch-Murnaghan equation of state [11]. The calculated values are listed in Table 1 and compared with available experimental and other theoretical studies. Our results are good agreement with other results.

<table>
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<tr>
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<th>a₀</th>
<th>B</th>
<th>B’</th>
<th>E₉</th>
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<td>4.18⁴ᵇ, 1.39ᵃ</td>
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<tr>
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<td></td>
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<tr>
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<td>49.6⁵</td>
<td>4.6¹⁴</td>
<td>1.2⁶</td>
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<tr>
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<td>-</td>
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<tr>
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<td>50.4²ᵉ, 54.1⁶ᵉ</td>
<td>4.0⁷ᵉ, 4.2⁵ᵉ</td>
<td>1.1⁷ᵃ</td>
</tr>
</tbody>
</table>

[⁶ᵃ, ¹²ᵇ, ³ᶜ, ¹³ᵈ, ²ᶜ, ¹⁴ᶠ, ¹⁵ᵍ, ¹ʰ]
Figure 2. Represents the total energy vs. cell volume for AlAs and AlSb compounds.

3.2 Electronic properties

The electronic band structure and total density of states of AlAs and AlSb compounds are calculated at their equilibrium volume. Figure 3 (a & b) presents the band structures in the first Brillouin zone along the high symmetry directions. Figure 3 (a & b) show that these compounds exhibit an indirect band gap at $\Gamma - X$ directions. The band gap values are listed in Table 1. It is in good agreement with other results. The zero energy corresponds to $E_F$. The lowest lying energy band is due to the anion s orbitals. Above this, from energy level -5 eV to 0 eV is mainly due to anion p orbitals and partial involvement of cation s orbitals. The bands above the Fermi level are mainly due to Al s orbitals. The valence band maximum is located at $\Gamma$ point and conduction band minimum is located at $X$ – point. The DOS profiles are also displayed in Figure 3 (c & d).

Figure 3. Represents the electronic band structure of (a) AlAs, (b) AlSb and total density of states of (c) AlAs (d) AlSb.
The optical properties of a solid are usually described by complex dielectric function $\varepsilon(\omega)$ and refractive index $n(\omega)$. The real and imaginary part of the dielectric function and the electron energy loss spectrum $L(\omega)$ is shown in Figures 4 (a, b and c). The spectrum of these compounds is radiated up to 13.5 eV. From the figure one can observed easily that the zero crossing of $\varepsilon_1(\omega)$ is located at 4.5 eV and 3.6 eV for AlAs and AlSb compounds. In the imaginary part $\varepsilon_2(\omega)$ the first peak is observed at 4.5 eV and 3.5 eV for AlAs and AlSb compounds, respectively. The electronic energy loss spectrum is related to the energy loss of electron transverse in the materials. The most prominent peak is located at 9.5 eV, 13.5 eV for AlAs and AlSb compounds, respectively.

Figure 4. Represents the real part $\varepsilon_1(\omega)$, imaginary part $\varepsilon_2(\omega)$ of (a) AlAs and (b) AlSb and electron energy loss spectrum $L(\omega)$ of (c) AlAs and AlSb compounds.

3.4 Bandgap Vs. Refractive index

In general the refractive index and dielectric constants of semiconductors represents their optical and electronic properties. Semiconductor devices require knowledge of the refractive index and band gap. In this work, the refractive index has been calculated using three different relations which are directly related to the fundamental bandgap of materials. The relations are following,

1. Moss atomic model relation [16],
   $$n = [\frac{K}{E_g}]^{\frac{1}{4}}$$
   where $n$ is the refractive index, $E_g$ is the band gap and $K (= 95 \text{ eV})$ is the attenuation index (or extinction coefficient).

2. Ravindra and Gupta [17] relation is,
   $$n = \alpha - \beta . E_g$$
   where $\alpha (= 4.16)$ and $\beta (= 0.85)$ are constants.

3. Herve and Vandamme’s empirical relation, based on oscillatory theory [18],
   $$n = \sqrt{1 + \left(\frac{A}{E_g + B}\right)^2}$$
   where $A$, $B$ are 13.6 eV and 3.4 eV respectively.

Figure 5 shows that the variation of the bandgap with refractive index in the three different relations. The results are good agreement with the experimental and other theoretical
results. From the figure one can observe easily that the refractive index is linear with the bandgap. These compounds have the positive refractive index values. The results would be possible to aid further development of electronic devices based on AlAs and AlSb compound.

Figure 5. Represents the bandgap Vs refractive index of (a) AlAs, (b) AlSb compounds

4. Conclusion

In this work, we have studied the electronic and optical properties of AlAs and AlSb compounds using ab initio calculations. We found that these compounds are indirect band gap semiconductors. We have also presented the dielectric function, energy loss spectrum and refractive index of these compounds. Our calculated results are good agreement with other results.

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