First-principles calculations of the structural, electronic and optical properties of cubic $B_xGa_{1-x}As$ alloys

M. Guemou a,*, B. Bouhafs b, A. Abdiche c, R. Khenata d, Y. Al Douri e, S. Bin Omran f

a Engineering Physics Laboratory, University Ibn Khaldoum of Tiaret, BP 78-Zaaroura, Tiaret 14000, Algeria
b Modelling and Simulation in Materials Science Laboratory, Physics Department, University of Sidi Bel-Abbes, 22000 Sidi Bel-Abbes, Algeria
c Department of Physics and Astronomy, Faculty of Science, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia
d Laboratoire de Physique Quantique et de Modélisation Mathématique (LPQM), Département de Technologie, Université de Mascara, 29000 Mascara, Algeria
e Applied Materials Laboratory, Research Center, University of Sidi Bel Abbes, 22000 Sidi Bel Abbes, Algeria
f Modelling and Simulation in Materials Science Laboratory, Physics Department, University of Sidi Bel-Abbes, 22000 Sidi Bel-Abbes, Algeria

A R T I C L E   I N F O
Article history:
Received 8 November 2011
Received in revised form 28 January 2012
Accepted 30 January 2012
Available online 3 February 2012

Keywords:
Density functional calculations are performed to study the structural, electronic and optical properties of technologically important $B_xGa_{1-x}As$ ternary alloys. The calculations are based on the total-energy calculations within the full-potential augmented plane-wave (FP-LAPW) method. For exchange-correlation potential, local density approximation (LDA) and the generalized gradient approximation (GGA) have been used. The structural properties, including lattice constants, bulk modulus and their pressure derivatives, are in very good agreement with the available experimental and theoretical data. The electronic band structure, density of states for the binary compounds and their ternary alloys are given. The dielectric function and the refractive index are also calculated using different models. The obtained results compare very well with previous calculations and experimental measurements.

2012 Elsevier B.V. All rights reserved.

A B S T R A C T

Density functional calculations are performed to study the structural, electronic and optical properties of technologically important $B_xGa_{1-x}As$ ternary alloys. The calculations are based on the total-energy calculations within the full-potential augmented plane-wave (FP-LAPW) method. For exchange-correlation potential, local density approximation (LDA) and the generalized gradient approximation (GGA) have been used. The structural properties, including lattice constants, bulk modulus and their pressure derivatives, are in very good agreement with the available experimental and theoretical data. The electronic band structure, density of states for the binary compounds and their ternary alloys are given. The dielectric function and the refractive index are also calculated using different models. The obtained results compare very well with previous calculations and experimental measurements.

© 2012 Elsevier B.V. All rights reserved.

1. Introduction

Over the past few years, much attention has been devoted to the boron compounds and their alloys which have a wide range of technological applications, due to their excellent physical properties that include low ionicities [1,2], short bond lengths, wide band gaps, high thermal conductivity and large resistivity [3–7].

The incorporation of boron into the standard III–V compounds may open pathways for band gap engineering in III–V alloys. Specifically, long-wavelength materials for solar cell absorber, coherent light emitter and detector devices may enrich the realm of III–V optoelectronic applications.

Experimentally, $B_Ga_{1-x}As$ alloy was successfully grown by both molecular beam epitaxy (MBE) and metal–organic chemical vapor deposition (MOCVD). This alloy is used for light emitters or detectors and solar cell applications [8,9], and is very required for high temperature applications [5] and electro-optical devices in the short-wavelength range of the visible spectrum. This alloy is also very advantageous as it is used in a highly radioactive environment because it has the ability to self-heal the damage caused by β radiation and convert them into electricity [10]. On the theoretical front, Szwachi and Boguszewachi [11] and Hart and Zunger [12] have reported on the electronic properties of $B_Ga_{1-x}As$ alloy using $ab$ initio molecular dynamics and full potential linearized augmented plane wave methods, respectively. Azzi et al. [13] investigated the optical band gap bowing of 18 III–V alloys containing boron, using the plane wave expansion non-norm conserving $ab$ initio Vanderbilt pseudo-potential method. Very recently, Murphy et al. [14] reported on the deviation from Vegard’s law in six ternary $M_NAs$ (M and N are B, Al, Ga and In) random alloys using the CASTEP (Cambridge Serial Total Energy Package) program.

In this work, we employed the full potential linearized augmented plane wave method with both local density approximation (LDA) and general gradient approximation (GGA) for the exchange-correlation energy to calculate the structural, electronic and optical properties of BAs and GaAs binary compounds and their ternary alloys. The calculations show that BAs and GaAs are indirect and direct band gap semiconductors, respectively. The semiconducting ($\Gamma-X$) and ($\Gamma-G$) band gaps for BAs and GaAs are found to be 1.41 and 1.20 eV, respectively. For cubic $B_Ga_{1-x}As$ alloy, a crossover between the direct ($\Gamma-G$) and indirect ($\Gamma-X$) band gaps is located at the concentration x equal to 0.77, resulting in indirect band gap ($\Gamma-X$) semiconductor beyond this concentration. From the band structure calculations, one can also remarks that $B_{0.25}Ga_{0.75}As$ alloy exhibits the

* Corresponding author. Tel.: +213 772609731.
E-mail address: guemoumained7@gmail.com (M. Guemou).

0921-4526/$ - see front matter © 2012 Elsevier B.V. All rights reserved.
doi:10.1016/j.physb.2012.01.132
small gap among the other alloys which motivate us to calculate their optical properties.

The paper is organized as follows. We briefly describe the method of calculation in Section 2, and then the results of our work are presented and discussed in Section 3. The work is concluded in Section 4.

2. Method of calculation

The calculation of the structural, electronic and optical properties of $B_xGa_{1-x}As$ was carried out with a self-consistent scheme by solving the Kohn–Sham equations, using a non-relativistic full potential linear augmented plane wave (FP-LAPW) method in the framework of the density functional theory (DFT) as implemented in the WIEN2K computer package [15]. The exchange-correlation contribution was described within the generalized gradient approximation (GGA) of Perdew–Burke–Ernzerhof (PBE96). In addition to this approximation the local density approximation (LDA) parameterized by Perdew–Wang was also applied for structural and electronic properties. In the FP-LAPW method, the space is divided into an interstitial region (IR) and non-overlapping muffin tin (MT) spheres centered at the atomic sites. In the IR region, the basis set consists of plane waves. Inside the MT spheres, the basis sets are described by radial solutions of the one particle Schrödinger equation (at fixed energy) and their energy derivatives multiplied by spherical harmonics. We used a parameter $R_{MT}K_{max}=7$ which determines the matrix size, where $R_{MT}$ denotes the minimum radius of the sphere in unit cell, and $K_{max}$ gives the magnitude of the largest $K$ vector in the plane wave expansion. The muffin tin radii of B, As and Ga are adopted to be 1.45, 2.1 and 2.2 Bohr, respectively. The integrals over the Brillouin zone are performed up to 100 k-points for the zinc blende binary compounds and 250 k-points for the ternary alloys in the irreducible Brillouin zone.

3. Results and discussions

3.1. Structural properties

In this section, we calculate the structural properties of the binary compounds BAs and GaAs and their ternary $B_xGa_{1-x}As$ alloys in the zinc blende (ZB) structure using GGA and LDA schemes. Then, we model the alloys at some selected compositions ($x=0$, 0.25, 0.5, 0.75 and 1) with ordered structures which are described in terms of periodically repeated supercells with eight atoms per unit cell. In order to obtain the equilibrium lattice constant and the bulk modulus for the binary compounds and their alloys, we performed the structural optimization by

![Fig. 1. Composition dependence of the calculated lattice constants of zinc blende $B_xGa_{1-x}As$ alloys.](image)

Table 1

<table>
<thead>
<tr>
<th>Composition</th>
<th>This work</th>
<th>Other theoretical studies</th>
<th>Experiments data</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>GGA</td>
<td>LDA</td>
<td></td>
</tr>
<tr>
<td>GaAs</td>
<td>5.76</td>
<td>5.6</td>
<td>5.57&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td></td>
<td>62.89</td>
<td>73.65</td>
<td>81.92&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td></td>
<td>4.74</td>
<td>4.33</td>
<td>4.67&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>$B_{0.25}Ga_{0.75}As$</td>
<td>5.6</td>
<td>5.46</td>
<td>5.4&lt;sup&gt;c&lt;/sup&gt;</td>
</tr>
<tr>
<td></td>
<td>71.12</td>
<td>85.27</td>
<td></td>
</tr>
<tr>
<td></td>
<td>4.61</td>
<td>4.56</td>
<td></td>
</tr>
<tr>
<td>$B_{0.5}Ga_{0.5}As$</td>
<td>5.38</td>
<td>5.27</td>
<td>5.32&lt;sup&gt;c&lt;/sup&gt;</td>
</tr>
<tr>
<td></td>
<td>80.79</td>
<td>100.68</td>
<td></td>
</tr>
<tr>
<td></td>
<td>4.28</td>
<td>4.75</td>
<td></td>
</tr>
<tr>
<td>$B_{0.75}Ga_{0.25}As$</td>
<td>5.12</td>
<td>5.05</td>
<td>5.1&lt;sup&gt;c&lt;/sup&gt;</td>
</tr>
<tr>
<td></td>
<td>102.97</td>
<td>124</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3.93</td>
<td>5.35</td>
<td></td>
</tr>
<tr>
<td>BAs</td>
<td>4.83</td>
<td>4.76</td>
<td>4.72&lt;sup&gt;e&lt;/sup&gt;</td>
</tr>
<tr>
<td></td>
<td>135.04</td>
<td>150.23</td>
<td>133&lt;sup&gt;g&lt;/sup&gt;</td>
</tr>
<tr>
<td></td>
<td>4.30</td>
<td>3.93</td>
<td>4.29&lt;sup&gt;g&lt;/sup&gt;</td>
</tr>
</tbody>
</table>

<sup>a</sup> Ref. [18].
<sup>b</sup> Ref. [19].
<sup>c</sup> Ref. [4].
<sup>d</sup> Ref. [16].
<sup>e</sup> Ref. [20].
<sup>f</sup> Ref. [21].
<sup>g</sup> Ref. [22].
<sup>h</sup> Ref. [23].
<sup>i</sup> Ref. [24].
minimizing the total energy with respect to the cell parameters and the atomic positions. The calculated total energies as a function of unit cell volume were fitted by Munaghan’s equation of state. Table 1 summarizes the results of our calculations and compares them with other experimental and theoretical predictions. Considering the general trend that GGA usually overestimates the lattice parameters, our GGA results of binary compounds are in reasonable agreement with the experimental and other calculated values [4,16–24]. As it can be seen that the calculated lattice parameter for GaAs (x = 0) is larger than those of BAs (x = 1); \(a_0(\text{BAs}) < a_0(\text{GaAs})\). Since the anion atom is the same in both compounds, this result can be easily explained by considering the atomic radii of Ga and B: \(R(\text{Ga}) = 1.35 \text{ Å}, R(\text{B}) = 0.85 \text{ Å}\), i.e. the lattice constant increases with increasing atomic size of the cation element. The bulk modulus value for BAs is larger than those of GaAs; \(B(\text{BAs}) > B(\text{GaAs})\); i.e. in inverse sequence to \(a_0\) in agreement with the well-known relationship between \(B\) and the lattice constants: \(B \propto V_0^{-1/3}\), where \(V_0\) is the unit cell volume.

Fig. 1 shows the variation of the calculated equilibrium lattice constants versus concentration (x) for \(B_xGa_{1-x}As\) alloys. The obtained results concerning the behavior of the variation of lattice constants versus concentration x, i.e. decrease from GaAs to BAs are in good agreement with the available theoretical results [14]. It is worth mentioning here that Murphy et al. [14] incorporate gallium atoms (Ga) in boron arsenide (BAs) compound. As shown in Fig. 1 it is clearly visible that the variation of the lattice constant versus composition shows a small deviation from Vegard’s law with an upward bowing parameter equal to \(-0.34 \text{ Å}\) for GGA and \(-0.35 \text{ Å}\) for LDA. The bowing parameters are determined by fitting the calculated values with a polynomial function. The physical origin of this deviation should be mainly due to the mismatches of the lattice constants of BAs and GaAs compounds.

Fig. 2 shows the composition dependence of the bulk modulus for the \(B_xGa_{1-x}As\) alloys. It is obvious from Fig. 2 that the values of the bulk modulus increase with the B concentration, meaning that the addition of boron to GaAs improve their hardness. A significant deviation from linear composition dependence (LCD) is observed with downward bowings equal to 66.52 GPa and 40.69 GPa for GGA and LDA, respectively. The large bowing values are also due to the significant mismatch of the bulk modulus of BAs and GaAs compounds.

3.2. Band structure and density of states

The incorporation of boron to the standard III–V material systems may expand the possibilities for band gap engineering of new semiconductor devices [25]. In this section we turn our attention to study the electronic properties of BAs, GaAs and their ternary alloys via calculating the energy band structure and the density of states. Figs. 3 and 4 display the calculated band structure of the cubic binary compounds and their ternary alloys along some high symmetry lines in the Brillouin zone within the GGA–PBE approximation. The zero energy is chosen to coincide with the top of the valence band. Our calculations show the conduction band minimum (CBM) is located at \(\Gamma\) point for GaAs and at \(X\) point for BAs. The valence band maximum (VBM) occurs at \(\Gamma\) point in both compounds, resulting in indirect (\(\Gamma\)–X) and direct (\(\Gamma\)–\(\Gamma\)) band gaps for BAs and GaAs, respectively. For the composition \(x = 0.25, 0.50\) and 0.75 the \(B_xGa_{1-x}As\) alloy is a direct band gap material (\(\Gamma\)–\(\Gamma\)). The computed direct (\(\Gamma\)–\(\Gamma\))
and indirect (Γ→X) band gap values within LDA and GGA approximations for BₓGa₁₋ₓAs alloy are summarized in Table 2, along with the available theoretical and experimental results. Our calculated results are in excellent agreement with the available experimental and theoretical data.

The variation of the composition (x) versus the direct (Γ→Γ) and indirect (Γ→X) band gaps with GGA approximation is shown in Fig. 5. A crossover between the direct (Γ→Γ) and indirect (Γ→X) band gaps is observed at a concentration of 0.77, resulting in an indirect band gap (Γ→X) for the alloy beyond this concentration. Through Fig. 5, one can remark that the direct band gap (Γ→Γ) decreases and the indirect band gap (Γ→X) increases smoothly up to x=0.3, and beyond x=0.5 the fundamental gap (Γ→Γ) increases rapidly.

We have also calculated the gap bowing by fitting the non-linear variation of the calculated direct and indirect band gaps in terms of concentration with a polynomial function.

The results are shown in Fig. 5 and found to obey the following relations:

\[ E_{\Gamma-\Gamma} = 1.255 - 3.986x + 5.80x^2 \]  \hspace{1cm} \text{(direct gap)}
\[ E_{\Gamma-X} = 1.544 + 0.732x - 0.88x^2 \]  \hspace{1cm} \text{(indirect gap)}

The values of \( E_g \) deviate from the linear behavior. This deviation is characterized by an upward–downward bowing parameters equal to 5.8 eV and −0.88 eV for (Γ→Γ) and (Γ→X) band gaps, respectively. Our calculated value of the bowing parameter for the direct band gap (Γ→Γ) is larger than that obtained by Azzi and co-workers (3.39 eV), using the pseudo-potential calculations [13].

Since the shift between the lattice parameters of GaAs and BAs is larger than 15%, one must expect an important disorder in the electronic and structural properties. The most important result is that the BₓGa₁₋ₓAs alloys show an indirect band gap for compositions more than 77%.
Table 2  
Summary of the band-gaps of GaAs, BAs compounds and ZB B0.5Ga0.5As alloys. The energy is given in eV.

<table>
<thead>
<tr>
<th>Composition</th>
<th>This work</th>
<th>Other theoretical studies</th>
<th>Experiments data</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaAs $E_{\Gamma-X}$</td>
<td>1.20</td>
<td>1.42&lt;sup&gt;a&lt;/sup&gt;</td>
<td>1.45&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>$E_{\Gamma-\Gamma}$</td>
<td>1.51</td>
<td>1.49&lt;sup&gt;c&lt;/sup&gt;</td>
<td>1.98&lt;sup&gt;c&lt;/sup&gt;</td>
</tr>
<tr>
<td>B0.25Ga0.75As $E_{\Gamma-X}$</td>
<td>0.65</td>
<td>1.41&lt;sup&gt;d&lt;/sup&gt;</td>
<td></td>
</tr>
<tr>
<td>$E_{\Gamma-\Gamma}$</td>
<td>0.95</td>
<td>1.44</td>
<td></td>
</tr>
<tr>
<td>B0.75Ga0.25As $E_{\Gamma-X}$</td>
<td>1.63</td>
<td>1.44</td>
<td></td>
</tr>
<tr>
<td>$E_{\Gamma-\Gamma}$</td>
<td>1.18</td>
<td>1.09</td>
<td></td>
</tr>
<tr>
<td>BAs $E_{\Gamma-X}$</td>
<td>3.21</td>
<td>3.34&lt;sup&gt;e&lt;/sup&gt;, 3.46&lt;sup&gt;f&lt;/sup&gt;</td>
<td>1.46&lt;sup&gt;g&lt;/sup&gt;</td>
</tr>
<tr>
<td>$E_{\Gamma-\Gamma}$</td>
<td>1.41</td>
<td>1.20&lt;sup&gt;i&lt;/sup&gt;, 1.45&lt;sup&gt;b&lt;/sup&gt;</td>
<td>0.67&lt;sup&gt;h&lt;/sup&gt;</td>
</tr>
</tbody>
</table>

<sup>a</sup> Ref. [26].  
<sup>b</sup> Ref. [18].  
<sup>c</sup> Ref. [24].  
<sup>d</sup> Ref. [4].  
<sup>e</sup> Ref. [27].  
<sup,f</sup> Ref. [16].  
<sup>g</sup> Ref. [28].  
<sup>h</sup> Ref. [19].  
<sup>i</sup> Ref. [29].

Fig. 5. Composition dependence of the GGA band gaps for B<sub>x</sub>Ga<sub>1-x</sub>As alloys.

To obtain a deeper insight into the electronic structure, we have also calculated the total and the partial atomic densities of states (TDOS and PDOS) for only BAs, GaAs and B0.25Ga0.75As alloys as a prototype. These are displayed in Fig. 6. The TDOS and PDOS are computed using GGA approximation with a mesh of 100 special K-points for B0.25Ga0.75As alloy and 250 special K-points for GaAs and BAs compounds. The TDOS and PDOS are able to identify the angular momentum character of the different regions. For GaAs, the electronic state is separated into three regions: lower valence band (LVB), upper valence band (UVB) and conduction band (CB). The lower valence band is dominated by As-4s, and the upper valence band by Ga-4s and As-4p states. The Ga-3d states contribute to the lowest valence bands. The first conduction band is mainly due Ga-4p states with a mixture of Ga and As-d states. Our results are in best agreement with other theoretical work [26]. The DOS spectrum of BAs compound also shows three regions, two valence regions (LVB and UVB) below the top of the valence band ($E_F$) and one conduction band (CB) above $E_F$. The lower valence band is dominated by As-4s, and the upper valence band by As-4p, with a few contributions of B-2s for the first peak and B-2p for the rest for this band. The conduction band is predominately formed by B-2s and As-4p with a small contribution of As-3d in the last of this band. A similar topological feature is observed in view on the diagram of B0.25Ga0.75As alloy with two valence band regions (LVB and UVB) below the energy level ($E_F$) and one conduction band (CB) above the Fermi level. The lower part (LVB) is dominated by a mixture of B-2p, Ga-4s and As-4s states. The upper part (UVB) and the conduction band are dominated by As-4p, Ga-4p and B-2s states. The Ga and As-3d states contribute also in these regions (UVB and CB).

3.3. Optical properties

The incorporation of boron into GaAs causes a reduction of the band gap [30] and may offer a new class of materials for optoelectronic devices. From Fig. 8, we can see that the minimum of the fitted band gap is at about $x=0.25$. In this section, we present a study of the optical properties of the binary BAs and GaAs and only B0.25Ga0.75As alloy because it has the minimum direct band gap compared to the other alloys.

The optical properties may be attracted from the knowledge of the complex dielectric function $\varepsilon(\omega)=\varepsilon_1(\omega)+i\varepsilon_2(\omega)$. $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ are the real and imaginary components of the dielectric function, respectively. The imaginary part $\varepsilon_2(\omega)$ is directly related to the electronic band structure and it can be computed by summing up all possible transitions from the occupied to the unoccupied states, taking into account the appropriate transition dipole matrix elements using the following expression [32]:

$$\varepsilon_2(\omega) = \frac{\epsilon^2\hbar}{8\pi^2\omega^2} \sum_{\mathbf{k}} \int_{BZ} (M_{\mathbf{k}}(k))_r^2 \delta(\omega_{\mathbf{k}}(k)-\omega) \text{d}^3k$$

(3)

The integral is over the first Brillouin zone. The momentum dipole elements: $M_{\mathbf{k}}(k)=\langle u_{\mathbf{k}}|\hat{\mathbf{r}}\nabla|u_{\mathbf{k}}\rangle$, where $\hat{\mathbf{r}}$ is the potential vector defining the electric field, are matrix elements for direct
transitions between valence-band $u_v(r)$ and conduction-band $u_c(r)$ states, and the energy and Planck; $\omega_{cv}(k) = E_{ck} - E_{vk}$ is the corresponding transition energy.

The real part $\varepsilon_1(\omega)$ can be derived from the imaginary part using the familiar Kramers–Kronig transformations:

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} \lim_{\varepsilon \to 0^+} \int_0^{\infty} \frac{\omega'\varepsilon_2(\omega')}{\omega'^2 - \omega^2} \, d\omega'$$

where $P$ implies the principal value of the integral. The knowledge of both real and imaginary parts of the frequency dependent dielectric function allows the calculation of important optical functions such as the refractive index $n(\omega)$ using the following expression:

$$n(\omega) = \left[ \frac{\varepsilon_1(\omega)}{2} + \sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} \right]^{1/2}$$

**Fig. 6.** Total and partial DOS of BAs, GaAs and $\text{B}_{0.25}\text{Ga}_{0.75}\text{As}$. 
We have also calculated the refractive index \( n \) using some empirical models:

1. Moss formula based on atomic model [33]:
\[
E_k n^4 = k
\]
(6)

2. Herve and Vandamme’s empirical relation [34]:
\[
n = \sqrt{1 + \left( \frac{A}{E_g} + B \right)^2}
\]
with \( A = 13.6 \text{ eV} \) and \( B = 3.4 \text{ eV} \).

3. Expression proposed by Ravindra et al. [35]:
\[
n = a + \beta E_g
\]
(8)
where \( a = 4.084 \) and \( \beta = 0.62 \).

The calculated optical constants of BAs, GaAs and \( \text{B}_0.25\text{Ga}_{0.75}\text{As} \) obtained using the FP-LAPW method and the different models, are

### Table 3
Calculated refractive index and dielectric constants for ZB \( \text{B}_{0.25}\text{Ga}_{0.75}\text{As} \), BAs and GaAs. Available experimental and theoretical data from the literature are also included for comparison.

<table>
<thead>
<tr>
<th>Composition</th>
<th>This work</th>
<th>Other theoretical experiments</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>FP-LAPW</td>
<td>Relation (7)</td>
</tr>
<tr>
<td>GaAs</td>
<td>( n = 3.47 )</td>
<td>( 3.12 )</td>
</tr>
<tr>
<td>( \varepsilon )</td>
<td>12.08</td>
<td>9.73</td>
</tr>
<tr>
<td>( \text{B}<em>{0.25}\text{Ga}</em>{0.75}\text{As} )</td>
<td>( n = 3.37 )</td>
<td>( 3.50 )</td>
</tr>
<tr>
<td>( \varepsilon )</td>
<td>11.4</td>
<td>12.25</td>
</tr>
<tr>
<td>BAs</td>
<td>( n = 3.07 )</td>
<td>( 3.0 )</td>
</tr>
</tbody>
</table>

\( a \) Ref. [31].
\( b \) Ref. [23].
\( c \) Ref. [16].
\( d \) Ref. [29].
\( e \) Ref. [36].

Fig. 7. Calculated refractive index; real and imaginary parts of the dielectric function of BAs (left panel) and GaAs (right panel).
summarized in Table 3. It is clearly seen that the calculated values are found to be in good agreement with the previous data.

Figs. 6 and 7 display the real and the imaginary parts of the dielectric function as well refractive index spectrum for a radiation up to 14 eV for binary BaS, GaAs compounds and their ternary B<sub>25</sub>Ga<sub>0.75</sub>As alloy. As it can be seen, the optical spectrum does not vary greatly from BaS to GaAs to B<sub>25</sub>Ga<sub>0.75</sub>As. This is attributed to the fact that the conduction bands’ features and the symmetries of the wave functions, which dictate the selection rules and are fully reflected in the Matrix Moment Elements, are somewhat similar. The overall profile of calculated spectra of the binary compounds is in fairly good agreement with previous theoretical calculations [29,37,38]. Our analysis of the imaginary part of the dielectric function shows that the first critical point...
occurs at 3.1 eV, 1.0 eV and 0.63 eV for BAs, GaAs and B_{25}Ga_{0.75}As, respectively. These points represent the direct optical transitions between the top of valence band and the bottom of conduction band at Γ point. One can remark that the main peak of imaginary part of GaAs and B_{25}Ga_{0.75}As is situated between two humps. The main peaks in the spectra are located at about 5.20 eV, 4.00 eV and 3.80 eV for BAs, GaAs and B_{25}Ga_{0.75}As, respectively.

4. Conclusions

We have applied an FP-LAPW method to study the structural, electronic and optical properties of BAs, GaAs compounds and their ternary B_{x}Ga_{1-x}As alloys in zinc blende structure. A summary of the key findings follows:

(1) The lattice constant of B_{x}Ga_{1-x}As alloys exhibits a negative deviation from Vegard's law with bowing parameter equal to −0.34. A large deviation of bulk modulus from LCD has been observed, this deviation is mainly due to the mismatch of the bulk modulus of BAs with GaAs.

(2) A transition from direct to indirect gap is predicted for B_{x}Ga_{1-x}As at the composition x = 0.77.

(3) Finally, the results obtained by our work are in good agreement with other experimental and previous data, and we concluded that B_{0.25}Ga_{0.75}As is the optimized material for optoelectronic applications by this weak band gap, among B_{x}Ga_{1-x}As alloys.

Acknowledgments

Authors R. Khenata and S. Bin-Omran extend their appreciations to the Deanship of Scientific Research at King Saud University for funding the work through the research group Project no. RPG-VPP-088.

References