Materials Sciences and Application, **2011, 2, 729-738**
doi:10.4236/msa.2011.27101 Published Online July 2011 (http://www.SciRP.org/journal/msa)

Structural and Electronic Properties Calculations of $Al_xIn_{1-x}P$ Alloy

Mohammed Ameri[1*], Ali Bentouaf[1], Mohammed Doui-Aici[2], Rabah Khenata[3,4], Fatima Boufadi[1], Amina Touia[1]

[1]Département de Physique, Faculté des Sciences, Université Djillali Liabès, Sidi-Bel-Abbés, Algérie; [2]Laboratory Applied Materials (AML), Research Center (Ex: CFTE), Route de Mascara, University of Sidi-Bel-Abbes, Algeria ; [3]Laboratoire Quantum Physics and Mathematical Modeling of Matter (M LPQ3), University de Mascara, Mascara, Algeria; [4]Department of Physics and Astronomy, Faculty of Science, King Saud University, Riyadh, Saudi Arabia.
Email: lttnsameri@yahoo.fr

Received December 23rd, 2010; revised March 21st, 2011; accepted May 3rd, 2011.

ABSTRACT

The equilibrium structure and the electronic properties of III-V zinc-blende AlP, InP semiconductors and their alloy have been studied in detail from first-principles calculations. A full-potential linear muffin-tin-orbital (FP-LMTO) method has been used in conjunction with both the local-density approximation (LDA) and the generalized-gradient approximation (GGA) to investigate the effect of increasing the concentration of aluminum on the structural properties such as the lattice constants and the bulk moduli. Besides, we report the concentration dependence of the electronic band structure, the direct-indirect band gap crossovers and bowing. Using the approach of Zunger and co-workers the microscopic origins of the gap bowing were also explained. A reasonable agreement is found in comparing our results with other theoretical calculations.

Keywords*: *AlP*, *InP*, *Semiconductors*, *FP-LMTO*, *Bowing*, *Alloys

1. Introduction

Understanding the electronic properties of semiconductor alloys plays a vital role in developing new technologies. The advantage of alloying is that the alloy properties, such as band gap, can be tuned by varying the alloy composition to meet the specific requirements of modern device applications [1-3]. With the advent of small-structure systems, such as quantum wells and superlattices, the effects of alloy compositions, size, device geometry, doping and controlled lattice strain can be combined to achieve maximum tenability [4].

$Al_xIn_{1-x}P$ alloy provides wide bandgap energy in the non-nitride III-V semiconductors and has been wide applied in electronic and photonic devices. The parent (binary) compounds such as aluminum phosphide (AlP) and indium phosphide InP, are non-centrosymmetric cubic semiconductors with zinc-blende structures based on the space group F43m [5,6]. Recently, these compounds have attracted a great deal of attention, [5-41] expecting fabrication of important electronic devices. Indeed, InP is a very promising material for solar cells and high-performance computing and communications [7-9]. Similarly, AlP, with the largest direct gap of the III-V compound semiconductors, is undoubtedly the most "exotic". Usually, this material is alloyed with other binary materials for applications in electronic devices such as light-emitting diodes (e.g. aluminium gallium indium phosphide) [10].

Motivated by the technological importance of these materials, III-phosphides have been the subject of various theoretical investigations, from empirical [42] to first principles based on the density functional theory (DFT) [43,44]. Most of these studies have been undertaken using the pseudo-potential [45] or the full-potential linearized-augmented plane wave (FP-LAPW) method which considered to be one of the most accurate methods for calculating the structural and the electronic properties of solids, within the local density approximation (LDA) [46] or the generalized gradient approximation (GGA) [47]. Nevertheless, to the best of our knowledge, the (FP-LMTO) method has not yet been used to study the structural and the electronic properties of $Al_xIn_{1-x}P$ alloy.

Below, we report the results obtained in the study of the variation of different structural and electronic parameters such as lattice constant, bulk modulus, band gap and effective masses with the alloy fraction using the

(FP-LMTO) method. In our calculations, we have adopted the "special quasirandom structures" (SQS) approach [48,49] which is based on the observation that (for any given composition) atomic disorder mainly affects the electronic properties of an alloy through the short-range atomic structure. In fact, Zunger and coworkers have introduced "SQS" approach by the principle of close reproduction of the perfectly random network for the first few shells around a given site.

The paper is divided in three parts. In Section 2, we briefly describe the computational techniques used in this study. The most relevant results obtained for the ground-state properties as well as the bandgap, optical bowing and effective masse are presented and discussed in Section 3. Finally, in Section 4 we summarize the main conclusions of our work.

2. Computational Details

The calculations reported here were carried out using the ab-initio full-potential linear muffin-tin orbital (FP-LMTO) method [50,51] as implemented in the Lmtart code [52]. The exchange and correlation potential was calculated using the local density approximation (LDA) [46] and the generalized approximation (GGA) [47]. This is an improved method compared to previous (LMTO) methods. The FP-LMTO method treats muffin-tin spheres and interstitial regions on the same footing, leading to improvements in the precision of the eingenvalues. At the same time, the FP-LMTO method, in which the space is divided into an interstitial regions (IR) and non overlapping muffin-tin spheres (MTS) surrounding the atomic sites, uses a more complete basis than its predecessors. In the IR regions, the basis functions are represented by Fourier series. Inside the MTS spheres, the basis functions are represented in terms of numerical solutions of the radial Schrödinger equation for the spherical part of the potential multiplied by spherical harmonics. The charge density and the potential are represented inside the MTS by spherical harmonics up to $l_{max} = 6$. The integrals over the Brillouin zone are performed up to 35 special ***k***-points for binary compounds and 27 special ***k***-points for the alloys in the irreducible Brillouin zone (IBZ), using the Blöchl's modified tetrahedron method [53]. The self-consistent calculations are considered to be converged when the total energy of the system is stable within 10^{-5} Ry. In order to avoid the overlap of atomic spheres the MTS radius for each atomic position is taken to be different for each case. Both the plane waves cut-off are varied to ensure the total energy convergence. The values of the sphere radii (MTS), number of plane waves (NPLW), used in our calculation are summarized in **Table 1**.

3. Results and Discussions

3.1. Structural Parameters

To investigate the structural properties of AlP and InP compounds and their alloys in the cubic structure, we have started our FP-LMTO calculation with the zinc-blende structure and let the calculation forces to move the atoms to their equilibrium positions. We have chosen the basic cubic cell as the unit cell. In the unit cell there are four C anions , three A and one B, two A and two B, and one A and three B cations, respectively, for $x = 0.25$, 0.50 and 0.75. For the considered structures, we perform the structural optimization by calculating the total energies for different volumes around the equilibrium cell volume V_0 of the binary AlP, InP compound and their alloy. The

Table 1. The plane wave number PW, energy cut-off (in Ry) and the muffin-tin radius (MTS) (in a.u.) used in calculation for binary AlP and InP and their alloy in zinc blende (ZB) structure.

	PW		E_{cut} total (Ry)		MTS (a.u)		
x	LDA	GGA	LDA	GGA		LDA	GGA
0	5064	12050	92.120	156.381	In	2.453	2.510
					P	2.357	2.412
0.25	33400	65266	131.543	197.867	Al	2.395	2.411
					In	2.395	2.411
					P	2.348	2.939
0.50	33400	65266	136.726	205.941	Al	2.349	2.393
					In	2.349	2.393
					P	2.303	2.346
0.75	33400	65266	142.279	215.299	Al	2.280	2.340
					In	2.280	2.340
					P	2.280	2.294
1	5064	12050	105.387	184.707	Al	2.248	2.264
					P	2.248	2.264

calculated total energies are fitted to the Murnaghan's equation of state [54] to determine the ground state properties such as the equilibrium lattice constant *a*, and the bulk modulus *B*. The calculated equilibrium parameters (*a* and *B*) are given in **Table 2** which also contains results of previous calculations as well as the experimental data. The lattice constants obtained within the LDA for the parent binary system InP and AlP are respectively 0.17 % and 0.03 % lower than the experimental value, while the corresponding bulk modulus are 0.7% and 1.2% larger than the experimental value, which is the usual level of accuracy of the LDA. When comparing the results obtained within GGA, the lattice constant are 2.6 % for InP and 1.6 % for AlP larger than the experimental values and the corresponding bulk modulus are 15.14% and 4.7% smaller than the corresponding experimental values. Hence it is safe to conclude that the LDA bulk modulus and lattice constants is in fact in better agreement with the experimental data than the GGA values. The calculated bulks modulus using both approximation LDA and GGA decreases in going from AlP to InP, suggesting the more compressibility for InP compared to that for AlP.

Usually, in the treatment of alloys when the experimental data are scare, it is assumed that the atoms are located at the ideal lattice sites and the lattice constants varies linearly with concentration *x* according to the so-called Vegard's law [55].

$$a\left(A_xB_{1-x}C\right) = x\,a_{AC} + (1-x)\,a_{BC} \qquad (1)$$

where a_{AC} and a_{BC} are the equilibrium lattice constants of the binary compounds AC and BC respectively, a ($A_xB_{1-x}C$) is the alloy lattice constant. However, the law was postulated on empirical evidence, several cases of both positive and negative deviations from this law have been documented [56,57]. Hence, it has been suggested in the literature that the deviation from Vegard's law can be represented by a quadratic expression:

$$a\left(A_xB_{1-x}C\right) = x\,a_{AC} + (1-x)\,a_{BC} - x\,(1-x)b \qquad (2)$$

where *b*, is the bowing parameter accounting for the deviation from linearity.

Figures 1 and **2**, show the variation of the calculated equilibrium lattice constants and the bulk modulus versus concentration *x* for $Al_xIn_{1-x}P$ alloy. Our calculated lattice constants were found to vary almost linearly following the Vegard's law [55] with a marginal upward bowing parameters equal to –0.07143 Å. In going from InP to AlP, when the Al-content increases, the values of the lattice parameters of $Al_xIn_{1-x}P$ alloy decrease. This is due to the fact that the size of the Al atom is smaller than that of the In atom. Oppositely, one can see from **Figure 2** that the value of the bulk modulus increases with the increase of Al concentration. The deviation of the GGA bulk modulus from the linear concentration dependence with a downward bowing equal to +21.9259 GPa. The bowing lattice parameters and the bulk modulus are found to be equal to –0.168 Å and +13.9569 GPa by using LDA approximation. In view on **Table 2**, it is clear

Table 2. Computed lattice parameter *a* and bulk modulus *B* compared to experimental and other theoretical values of AlP and InP and their alloy.

	Lattice constant a(Å)				Bulk modulus *B*(GPa)			
	this work.		exp.	other calc.	this work.		exp.	other calc.
	LDA	GGA			LDA	GGA		
x								
0	5.8509	6.014	5.861[b] ,5.8686[e]	5.942[a],5.688[c],5.869[d] ,5.8783[g],5.729[h],5.838[l] ,5.968[l] ,5.729[m],5.930[n] ,5.6591[o] ,5.93[s]	71.5399	60.25	71[b]	68[a],70[c],73.26[g] ,73.60[h] ,71[l] ,62[l] ,74[m] ,76[n] ,76[s]
0.25	5.7979	5.9092			73.2808	61.4585		
0.5	5.687	5.7922			75.7209	65.5753		
0.75	5.5749	5.6649			80.2789	72.4857		
1	5.449	5.534	5.451[e] ,5.467[i]	5.471[c] ,5.462[d] ,5.44285[g] ,5.41700[h],5.508[j],5.42[k] ,5.520[n] ,5.4131[o] ,5.43[p] ,5.40[q] ,5.48[r]	87.067	81.89	86[f]	84.5[c],95.46[g],88.60[h] ,81.52[j] ,86.5[k] ,89[l] 90,46[p] ,90[q] ,88[r]

[a]Ref. [11]; [b]Ref. [12]; [c]Ref. [13]; [d]Ref. [14]; [e]Ref. [17]; [f]Ref. [18]; [g]Ref. [19]; [h]Ref. [20]; [i]Ref. [23]; [j]Ref. [24]; [k]Ref. [25]; [l]Ref. [26]; [m]Ref. [27]; [n]Ref. [29]; [o]Ref. [31]; [p]Ref. [32]; [q]Ref. [33]; [r]Ref. [34]; [s]Ref. [39].

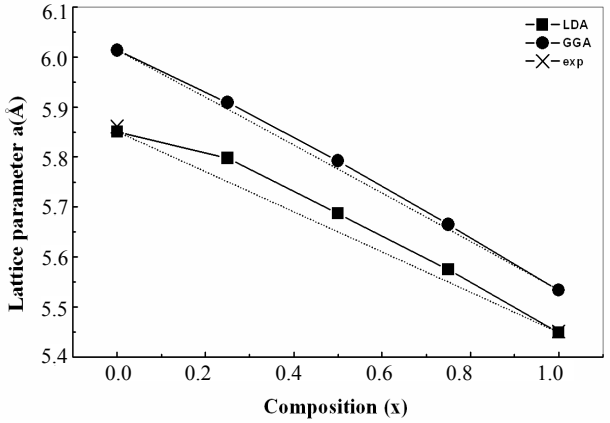


Figure 1. Composition dependence of the calculated lattice constants within GGA (solid circle) and LDA (solid squares) of $Al_xIn_{1-x}P$ alloy compared with Vegard's prediction (dot line).

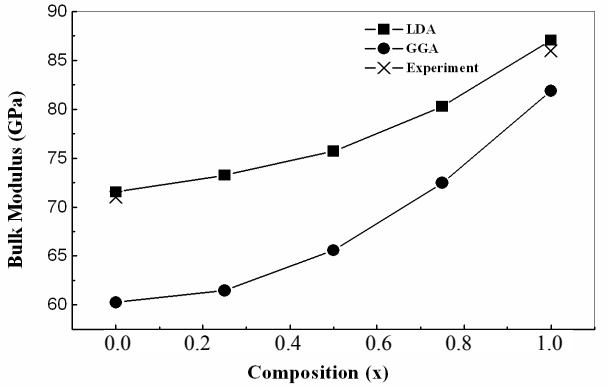


Figure 2. Composition dependence of the calculated bulk modulus within GGA (solid circle) and LDA (solid squares) $Al_xIn_{1-x}P$ alloy.

that the LDA yields higher values than the experiment while GGA provides a good agreement.

3.2. Electronic Properties

The important features of the band structure (direct Γ-Γ and indirect Γ-X band gaps) are given in **Table 3**. It is clearly seen that the band gaps are on the whole underestimated in comparison with experiments results. This underestimation of the band gaps is mainly due to the fact that both the simple form of LDA or GGA do note take into account the quasiparticle self energy correctly [58] which make them not sufficiently flexible to accurately reproduce both exchange and correlation energy and its charge derivative. We worth also mention that in general, it is far to say that the experimental data are well reproduced by the calculation. On raison for this difference is that in our calculations we have assumed the crystal to be at $T = 0$ *K* and thus do not include contributions from lattice vibrations that are present at room temperature measurements. The calculated band gaps for AlP compound and in good agreement with the available theoretical results. This agreement disappears for the case of InP compound. **Figure 3** shows the plots of the concentration variation of the direct gap (Γ–Γ) and indirect gap (Γ-X) the studied alloys within both LDA and GGA. Increasing Al content leads to a shift of the conduction band (CB) upwards the Fermi energy (E_F) resulting an increase of the direct energy band gap (Γ–Γ). The calculated direct band gap values are 0.56 (0.26), 1.0 (0.83), 1.58 (1.45), 1.75 (1.74) and 3.36 (3.08) eV within of LDA (GGA) approach for x = 0.0, 0.25, 0.5, 0.75 and 1.0, respectively. The band structure calculations in the present work yield a direct gap (Γ–Γ) for InP, while for AlP compound an indirect gap (Γ–X) has been determined. Hence, one can expect that the band gap of $Al_xIn_{1-x}P$ alloys should undergo a crossover between the direct and the indirect band in going from x = 0 to x = 1. As shown in **Figure 3**, this crossover occurs at x = 0.79 for LDA and at 0.82 for GGA. For both approximation the predicted crossover value is twice larger that those determined by Onton and co-authors [59].

The calculated band gap versus concentrations was fitted by a polynomial equation.

$$E_g(x) = xE_{AC} + (1-x)E_{BC} - bx(1-x) \qquad (3)$$

where E_{AC} and E_{BC} corresponds to the of the AlP and InP gaps for the $Al_xIn_{1-x}P$ alloy. The results are shown in **Figure 3** and are summarized as follows:

$$\begin{cases} E_{\Gamma-\Gamma} = 0.68 + 0.056x + 2.41x^2 & \text{(LDA)} \\ E_{\Gamma-X} = 1.56 + 4.12x - 4.05x^2 & Al_xIn_{1-x}P \end{cases} \qquad (4)$$

$$\begin{cases} E_{\Gamma-\Gamma} = 12.96 - 4.01x + 1.39x^2 & \text{(GGA)} \\ E_{\Gamma-X} = 1.73 + 3.81x - 3.69x^2 \end{cases}$$

It is clear from the above equations that the direct (Γ → Γ) and indirect (Γ → X) band gaps versus concentration have a nonlinear behavior. The direct gap (Γ → Γ) has a downward bowing with a value of 1.396, while the indirect gap (Γ → X) has an upward bowing of –3.907. These parameters are lower than those obtained using the LDA (2.38 and –4.059).

The physical origins of gap bowing were investigated following the approach of Zunger and co-workers [60], which decompose it into three contributions. The overall bowing coefficient at a given average composition *x* measures the change in the band gap according to the formal reaction

$$x\ \mathrm{AC}(a_{AC}) + (1-x)\ \mathrm{BC}\ (a_{BC}) \rightarrow A_xB_{1-x}C\ (a_{eq}) \qquad (5)$$

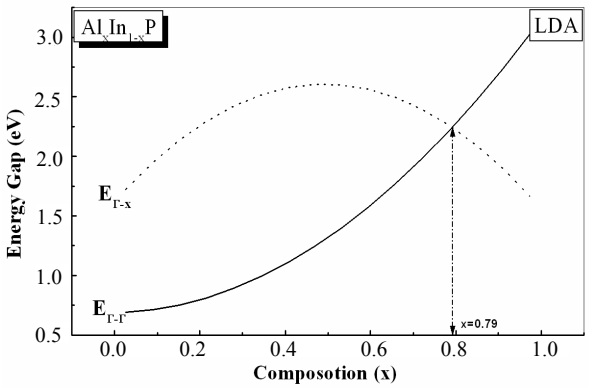
where a_{AC} and a_{BC} are the equilibrium lattice constant

Table 3. Direct band gap energy of $Al_xIn_{1-x}P$ alloys at different Al concentrations (all values are in eV).

	Energy gap (eV) (Γ-Γ)				Energy gap (eV) (Γ-X)			
	this work.		exp.	other calc.	this work.		exp.	other calc.
	LDA	GGA			LDA	GGA		
x								
0	0.5647	0.2674	1.39[c], 1.35[d], 1.424[l], 1.350[m]	1.39[a],1.98[e],1.23[f], 1.54[g],1.67[h],0.62[j] ,0.85[j],1.50[j],1.232[k], 1.3831[n],1.34[r]	1.6479	1.8804		0. 43[g] ,1.5522[n], 2.19[r]
0.25	1.0099	0.8315			2.3836	2.7014		
0.5	1.5819	1.4578			2.3997	2.5271		
0.75	1.578	1.742			2.5961	2.7014		
1	3.3666	3.0881	3.63[b], 2.45[d]	3.44[a],2.54[e] ,3.26[f] , 2.55[g] ,3.073[i], 3.3457[n], 3.11[o] ,3.62[p] ,3.073[q]	1.4658	1.6386	2.50[b], ,2.52[s] ,2.500[l]	2.17[a],1.44[g],1.635[i], ,1.44[j],1.57[j],2.50[j] ,1.4194[n],1.41[o],1.49[t] ,2.50[p],1.635[q]

[a]Ref. [14]; [b]Ref. [15]; [c]Ref. [16]; [d]Ref. [17]; [e]Ref. [19]; [f]Ref. [20]; [g]Ref. [21]; [h]Ref. [22]; [i]Ref. [24]; [j]Ref. [26]; [k]Ref. [27]; [l]Ref. [28]; [m]Ref. [30]; [n]Ref. [31]; [o]Ref. [32]; [p]Ref. [36]; [q]Ref. [37]; [r]Ref. [38]; [s]Ref. [23]; [t]Ref. [35]

lattice constant of the alloy with the average composition *x*.



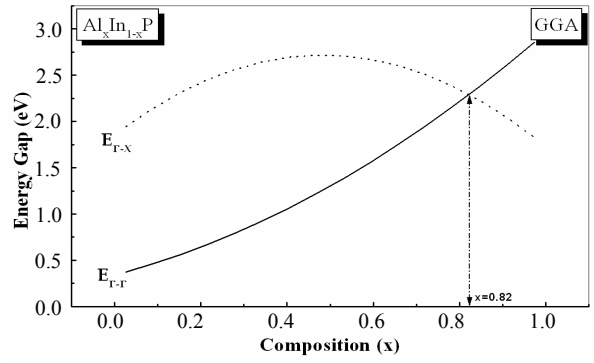


Figure 3. Energy band gap of $Al_xIn_{1-x}P$ alloy as a function of Al composition using LDA and GGA approximations.

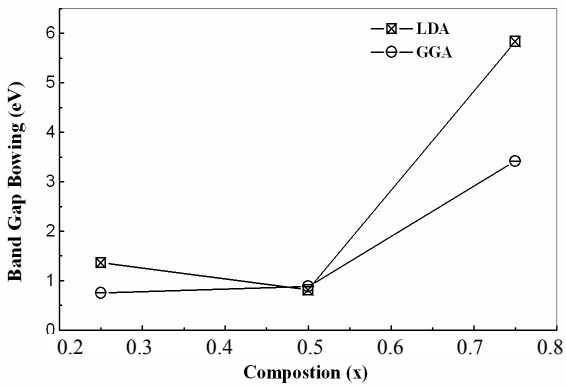


Figure 4. Calculated optical bowing parameter as a function of composition v*x* within LDA (xCenter Square) and GGA (-Center circle).

The Equation (5) is decomposed into three steps:

$$\mathrm{AC}(a_{AC}) + \mathrm{BC}\ (a_{BC}) \rightarrow AC\ (a) + BC\ (a) \qquad (6)$$

$$x\ \mathrm{AC}(a) + (1-x)\ \mathrm{BC}\ (a) \rightarrow A_xB_{1-x}C\ (a) \qquad (7)$$

$$A_xB_{1-x}C\ (a) \rightarrow A_xB_{1-x}C\ (a_{eq}) \qquad (8)$$

The first step measures the volume deformation (VD) effect on the bowing. The corresponding contributions b_{VD} to the bowing parameter represents the relative response of the band structure of the binary compounds AC and BC to hydrostatic pressure, which here arises from the change of their individual equilibrium lattice constants to the alloy value $a = a(x)$. The second contribution,

the charge exchange (CE) contribution b_{CE}, reflects the charge transfer effect which is due to the different (averaged) bonding behavior at the lattice constant a. The final step measures changes due to the structural relaxation (SR) in passing from the unrelaxed to the relaxed alloy by b_{SR}. Consequently, the total bowing parameter is defined as

$$b = b_{VD} + b_{CE} + b_{SR}. \quad (9)$$

The general representation of the composition-dependent band gap of the alloys in terms of binary compounds gaps of the, $E_{AC}(a_{AC})$ and $E_{BC}(a_{BC})$, and the total gap bowing parameter b is defined as:

$$E_g(x) = xE_{AC}(a_{AC}) + (1-x)E_{BC}(a_{BC}) - bx(1-x) \quad (10)$$

This allows a division of the total gap bowing b into three contributions according the following expressions:

$$b_{VD} = \frac{E_{AC}(a_{AC}) - E_{AC}(a)}{1-x} + \frac{E_{BC}(a_{BC}) - E_{BC}(a)}{x} \quad (11)$$

$$b_{CE} = \frac{E_{AC}(a)}{1-x} + \frac{E_{BC}(a)}{x} - \frac{E_{ABC}(a)}{x(1-x)} \quad (12)$$

$$b_{SR} = \frac{E_{ABC}(a) - E_{ABC}(a_{eq})}{x(1-x)} \quad (13)$$

All terms presented in Equations (11)-(13) are computed separately via self-consistent band structure calculations. The different contributions to the gap bowing were calculated using the LDA and the GGA schemes and the results are given in **Table 4**. The calculated band gap bowing coefficient for random $Al_xIn_{1-x}P$ alloy ranges from 1.3614 eV (x = 0.25) to 5.8396 (x = 0.75). Our result for x = 0.5 is higher than the experimental one and is in excellent agreement with those obtained by Ferhat and co-authors [61] using the full potential linearized augmented plane wave. One can note that for x = 0.25 and 0.50 the main contribution to the gap bowing is due to the volume deformation (VD) effect. The importance of b_{VD} can be correlated with the mismatch of the lattice constants of the corresponding binary compounds. Consequently, the main contribution to the gap bowing is raised from the volume deformation effect. In the case of x = 0.75, the contribution of the charge transfer b_{CE} has been found greater than those of the volume deformation b_{VD}. This contribution is due to the different electronegativities of the In and Al or P atoms. Indeed, b_{CE} scales with the electronegativity mismatch. The contribution of the structural relaxation is negligible and the band gap bowing is due essentially to the charge exchange effect. Finally, it is clearly seen that our LDA values for bowing parameters are larger than the corresponding values within GGA.

3.3. Calculated Effective Masses

The knowledge of the electron and hole effective mass values is indispensable for the understanding of transport phenomena, exciton effects and electro-hole in semiconductors. Therefore, it would be of much interest to determine the electron and hole effective mass values for the alloys for various Al content. We have computed the electron effective mass at the conduction band minima (CBM) and hole effecRtive mass at the valence band maxima (VBM) for the studied alloy. The electron and hole effective masses values are obtained from the curvature of the energy band near the Γ-point at the CBM and VBM for all concentration. At the Γ-point the s-like conduction band effective mass can be obtained through a simple parabolic fit using the definition of the effective mass as the second derivative of the energy band with respect to the wave vector, k, via:

$$m^*/m_0 = (\hbar^2/m_0) \cdot 1/(\partial^2 E/\partial k^2) \quad (14)$$

Table 4. Decomposition of optical bowing into volume deformation (VD), charge exchange (CE) and structural relaxation (SR) contributions (all values in eV).

		this work.		exp	other cal.
		LDA	GGA		
x					
0.25	b_{VD}	0.6354	0.6873		
	b_{CE}	–0.0756	–0.1583		
	b_{SR}	0.8016	0.2234		
	b	1.3614	0.7524		
0.5	b_{VD}	–0.039	0.7376		0.740[b]
	b_{CE}	0.986	–0.09087		0.265[b]
	b_{SR}	–0.1312	0.2333		–0.172[b]
	b	0.815	0.880	0.38[a], 0.568[a]	0.834[b]
0.75	b_{VD}	0.7286	0.7941		
	b_{CE}	5.2214	2.6625		
	b_{SR}	–0.1104	–0.0399		
	b	5.8396	3.4167		

[a]Ref. [40]; [b]Ref. [61]

Table 5. Electron (m_e^*), light hole (m_{lh}^*) and heavy hole (m_{hh}^*) effective mass (in units of free electron mass m_0) of the ternary alloys under investigation compared with the available experimental and theoretical predictions.

	m_{lh}^*			m_{hh}^*			m_{lh}^*		
	this work.		other calc.	this work.		other calc.	this work.		other calc.
x	LDA	GGA		LDA	GGA		LDA	GGA	
0	0.004	0.032	0.095[a], 0.058[a]	0.351	0.603	0.389[a], 0.477[a]	0.098	0.103	0.093[a], 0.057[a]
			0.570[b], 0.060[b]			0.430[b], 0.400[b]			0.097[a], 0.078[a]
			0.079[b], 0.081[b]			0.47[b], 0.895[a]			0.104[b], 0.118[b]
						0.520[b],0.610[b]			0.052[a], 0.074[a]
						0.970[b], 0.90[b]			0.051[a]
						0.63[b], 0.950[b]			
0.25	0.0042	0.047		0.804	0.770		0.219	0.367	
0.50	0.032	0.042		4.126	0.7648		4.214	0.2602	
0.75	0.0427	0.0428		0.857	0.8448		0.269	0.2870	
1	0.167	0.024	0.176[a], 0.170[a]	0.462	6.194	0.489[a], 0.509[a]	0.159	0.182	0.187[a], 0.181[a]

[a]Ref. [31]; [b]Ref. [41]; [c]Ref. [62]

where m^* is the conduction electron effective mass and m_0 is the free electron mass. We can calculate the curvature of the valence band maximum using the following approach: if the spin-orbit interaction were neglected, the top of the valence band would have a parabolic behavior; this implies that the highest valence bands are parabolic in the vicinity of the Γ-point. In this work, all the studied systems satisfy this parabolic condition of the valence band maximum at the Γ-point. Within this approach, and by using the appropriate expression of Equation (14) (using a plus sign instead of the minus sign in the prefactor), we have computed the effective masses of the heavy and light holes at the Γ-point. The calculated electron and hole effective mass values for the parent binary compounds InP and AlP and their alloy are given in **Table 5**. Results from earlier theoretical works are also quoted for comparison. Our results for the binary compounds are in fairly good agreement with the available theoretical data. We would like mentioning here that the divergence of some values should be expected since the computation of the effective mass is very sensitive to the form of the energy band. The highest curvature of the electronic band yields the smallest effective mass of the charge carriers and the highest conductivity. From **Table 5** data, we can outline that holes are much heavier than electrons, for all concentrations in $Al_xIn_{1-x}P$ alloy, so carrier transport in this alloy should be dominated by electrons.

4. Conclusions

We have performed first-principles calculations using (FP-LMTO) method within the LDA and GGA for the zinc-blende $Al_xIn_{1-x}P$ alloy (x = 0.0; 0.25; 0.50; 0.75; 1.00). We have found that lattice parameter follows Vegard's law, the bulk modulus varies significantly with the composition x and the electronic band structure has a nonlinear dependence on the composition. We have characterized the deviation from the linear behavior by calculating the optical bowing parameter. The main contribution to the total bowing parameter arises from structural (volume deformation) and chemical effects. The computed effective masses of the systems studied are found comparable to those reported in literature. Our results provide an estimate of this important compound.

5. Acknowledgements

The author Rabah KHENATA extends his appreciation to the Deanship of Scientific Research at King Saud University for funding the work through the research group project No RGP-VPP-088.

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