



Bismuth in gallium arsenide: Structural and electronic properties of GaAs_{1-x}Bi_x alloys

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ABSTRACT

The structural and electronic properties of cubic GaAs_{1-x}Bi_x alloys with bismuth concentration 0.0, 0.25, 0.50, 0.75 and 1.0 are studied using the 'special quasi-random structures' (SQS) approach of Zunger along with the generalized gradient approximation (GGA) and the Engel–Vosko generalized gradient approximation (EV-GGA). The lattice constant, bulk modulus, derivative of bulk modulus and energy gap vary with bismuth concentration nonlinearly. The present calculations show that the band gap decreases substantially with increasing bismuth concentration and that spin–orbit coupling influences the nature of bonding at high Bi concentrations.

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1. Introduction

III–V Bi doped ternary alloys such as GaAs_{1-x}Bi_x have attracted a great deal of interest due to their significant potential applications in solar cells, optoelectronic devices, semiconductor lasers and optical detectors [1]. Doping GaAs with Bi is found to have a significant influence on electronic and optical properties. Madouri et al. [2] have observed a huge reduction in the band gap by replacing As with Bi. Ever since this discovery, there has been an intensive effort devoted to the understanding the effect of Bi on the electronic properties of GaAs. The size of the Bi atom is large compared to that of As atom. Hence when Bi atom replaces As atom substitutionally, a compressive strain develops in the crystal [3–5]. As a result, the electronic properties of the pristine compound are modified. The large reduction in band gap is thought to be due to a resonant interaction between the Bi 6p state and the valence band maximum [6,9].

In 2006 Young [6] was able to successfully use the methods of surfactant technology to introduce Bi in GaAs [7]. This was significantly different from the typical GaAs growth conditions in molecular beam epitaxy (MBE) [8]. GaAsBi is a nonconventional alloy in the sense that the alloying element Bi introduces bound states in addition to bands, and behaves more like an isoelectronic

donor (Bi) rather than a true alloying element [6,9]. The growing demand for new technologies coupled with the unusual properties of these materials provides the motivation for the current study. In this paper a structural and electronic properties of the GaAs_{1-x}Bi_x ternary alloys are studied using the density functional theory (DFT). Calculations are performed with and without spin–orbit coupling (SOC). By varying the composition of bismuth, we hope to throw light on the effect of additional Bi. We have used the generalized gradient approximation (GGA) for the exchange and correlation potential and the Engel–Vosko generalized gradient approximation (EVGGA). Our calculations differ from those of previous calculations [2,32] in the sense that we use the 'special quasi-random structures' (SQS) approach of Zunger et al. [10]. We present the actual values of the band gaps, while in the previous calculations [2,32] the reported band gaps were scissors' corrected. Hence the gaps, which they quote, are exactly the same as the experimental gaps.

The rest of the paper is organized as follows: Section 2 is devoted to the method of calculation. The results and discussion are presented in Section 3 and Section 4 summarizes the main results of our calculations.

2. Method of calculation

The total energy calculations are performed for GaAs_{1-x}Bi_x for $x=0.0, 0.25, 0.5, 0.75$ and 1.0 with and without spin–orbit coupling (SOC). In this work, we have used the 'special quasi-random

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structures' (SQS) approach of Zunger et al. [10] to reproduce the randomness of the alloys for the first few shells around a given site. This approach is reasonably accurate to describe the physical properties that are not affected by the errors introduced using the concept of periodicity beyond the first few shells.

The calculations were carried out using the full potential linearized augmented plane wave (FP-LAPW) method as implemented in WIEN2K code [11]. The exchange correlation potential was treated using the generalized gradient approximation (GGA) [12] for the self-consistent calculations. We have also used the

Engel–Vosko GGA (EVGGA) formalism [13] for band structure calculations. The latter approximation is used to overcome the underestimation of the energy gap in both LDA and GGA of underestimation the energy gap [14]. This shortcoming is ascribed to the fact that LDA and GGA do not reproduce the exchange correlation energy and its charge derivative correctly. The EVGGA is a modified form of GGA, which is able to better reproduce the exchange potential at the expense of less agreement in the exchange energy, resulting in a better band splitting. However, the calculations of quantities that depend on an

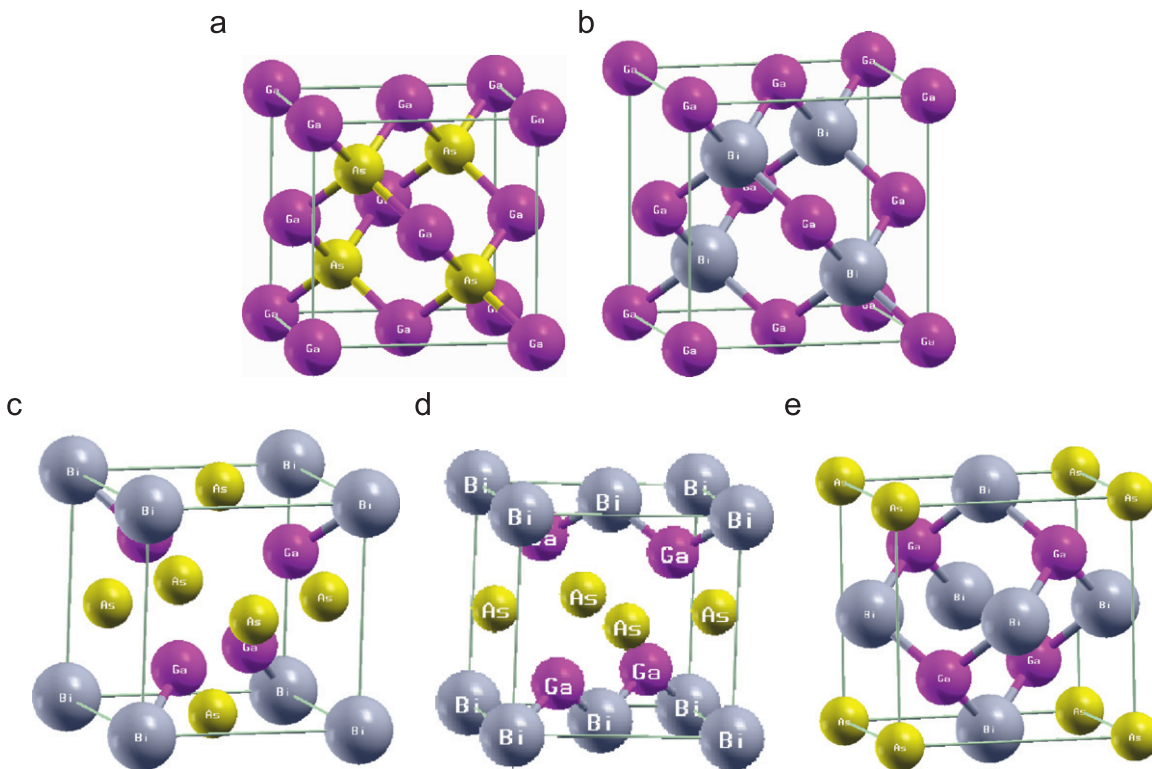


Fig. 1. Crystal structure of the binary and ternary alloys $\text{GaAs}_{1-x}\text{Bi}_x$; (a) 0.0, (b) 0.25, (c) 0.5, (d) 0.75 and (e) 1.0.

Table 1

Calculated lattice constants a (Å), bulk modulus B_0 (GPa) and derivative of bulk modulus B' values with GGA-approximation with and without spin-orbit coupling along with other experimental and theoretical values for $\text{GaAs}_{1-x}\text{Bi}_x$.

x	Lattice parameter a (Å)			Bulk modulus (GPa)	Bulk modulus derivative
	Our work	Exp.	Other calc.		
$\text{GaAs}_{1-x}\text{Bi}_x$ (without spin-orbit coupling)					
0	5.75	5.65 ^a	5.76 ^b , 5.62 ^c	61.78, 71.78 ^c	4.43, 4.64 ^c
0.25	6.19		6.04 ^b , 5.81 ^c	37.94, 62.22 ^c	5.15, 4.04 ^c
0.50	6.34		6.20 ^b , 5.99 ^c	35.67, 53.98 ^c	3.75, 4.63 ^c
0.75	6.40		6.33 ^b , 6.15 ^c	35.21, 46.63 ^c	4.86, 4.57 ^c
1	6.45	6.32 ^{a,d}	6.44 ^e , 6.30 ^c , 6.27 ^c , 6.17 ^e , 6.28 ^f	36.92, 43.25 ^c , 46.26 ^c , 46.10 ^e , 46.37 ^f	4.56, 4.84 ^c , 4.37 ^c , 4.57 ^e , 4.43 ^f
$\text{GaAs}_{1-x}\text{Bi}_x$ (with spin-orbit coupling)					
0	5.75	5.65 ^a		61.48	4.31
0.25	6.20			37.76	4.71
0.50	6.36			34.15	1.67
0.75	6.44			31.15	5.00
1	6.52	6.32 ^{a,d}		31.06	4.20

^a Ref. [29].

^b Ref. [2].

^c Ref. [31].

^d Ref. [30].

^e Ref. [32].

^f Ref. [33].

accurate description of the exchange potential as the equilibrium volume and bulk modulus using EVGGA are in poor agreement with experiment [14].

The spherical harmonics inside non-overlapping muffin-tin (MT) spheres surrounding the atomic are expanded up to $l_{max}=10$. The muffin-tin radii are 1.6 a.u. (a.u.) for Bi, whereas a 1.95 a.u. is used for both Ga and As. The plane wave cut-off of $K_{max}=7.0/R_{MT}$ was chosen for the expansion of the wavefunctions in the interstitial region for the binary compounds GaAs, GaBi and ternary alloys $GaAs_{1-x}Bi_x$. The charge density was Fourier expanded up to $G_{max}=14$ (Ryd) $^{1/2}$. The irreducible wedge of the Brillouin zone was described by a mesh of 35 special k -points for binary compounds and alloys except for the case of $x=0.5$, where we used a mesh of 64 special k -points. In the case of band structure calculations, we used denser meshes of 220 k -points for binary as well as ternary alloys of $x=0.25$ and 0.75 , whereas 216 k -points were used for $x=0.5$. The self-consistent calculations are converged since the total energy of the system is stable within 10^{-5} Ry.

3. Results and discussion

3.1. Structural properties

In this section, we present the structural properties of the $GaAs_{1-x}Bi_x$ compounds for compositions $x=0.0, 0.25, 0.5, 0.75$ and 1.0 . The binary alloys, GaBi and GaAs, are described by zinc-blende structure, whereas the ternary alloys are modeled using the SQS approach [10]. For the composition $x=0.25$ and 0.75 the simplest structure is an eight-atom simple cubic lattice (luzonite): the cations with the lower concentration form a regular simple cubic lattice. For $x=0.5$, the smallest ordered structure is (001) supercell (see Fig. 1). The structures of all the compounds were optimized by calculating the total energy as a function of volume, which was followed by fitting the results with Murnaghan's equation of state [15]. From this fitting, we obtained the optimum lattice constant and bulk modulus. Table 1 presents our calculated values obtained after optimization compared with the available experimental data and other theoretical calculations. We have performed calculations with and without SOC, which is very important for Bi. The optimized lattice constants deviate from those estimated by Vegard's law [16]. According to Vegard's law [16],

$$a(AB_{1-x}C_x) = xa_{AC} + (1-x)a_{AB} \quad (3.1)$$

where a_{AC} and a_{AB} are the equilibrium lattice constants of the binary compounds AC and BC, respectively, and $a(AB_{1-x}C_x)$ is the alloy lattice constant. The relation of the lattice constant exhibits a quadratic term as a result of the mismatch between the lattice constants of the extreme binary alloys, AB and AC. Therefore, the lattice constant is better described as follows:

$$a(AB_{1-x}C_x) = xa_{AC} + (1-x)a_{AB} - x(1-x)b \quad (3.2)$$

Here, the constant b is the bowing parameter. The bowing parameter for $GaAs_{1-x}Bi_x$ compounds is -1.00 (without SOC) and -0.93 (with SOC), where the negative sign indicates the increase in lattice constant from GaAs \rightarrow GaBi presented in Fig. 2(a), using the GGA approximations. This observation agrees well with the experimental observation of Oe and Okamoto [17]. The variation of bulk modulus with Bi concentration shows that a decreasing change of $GaAs_{1-x}Bi_x$ alloys is consistent (from GaAs \rightarrow GaBi) with bowing parameter $+60.46$ (without SOC) and 54.72 (with SOC) see Fig. 2(b). In Fig. 2, we observe that for concentrations up to 25% of Bi there is no obvious change in the lattice parameter as well as in bulk modulus by adding SOC. This could be due the low concentration of Bi. But at higher concentration of Bi the bowing

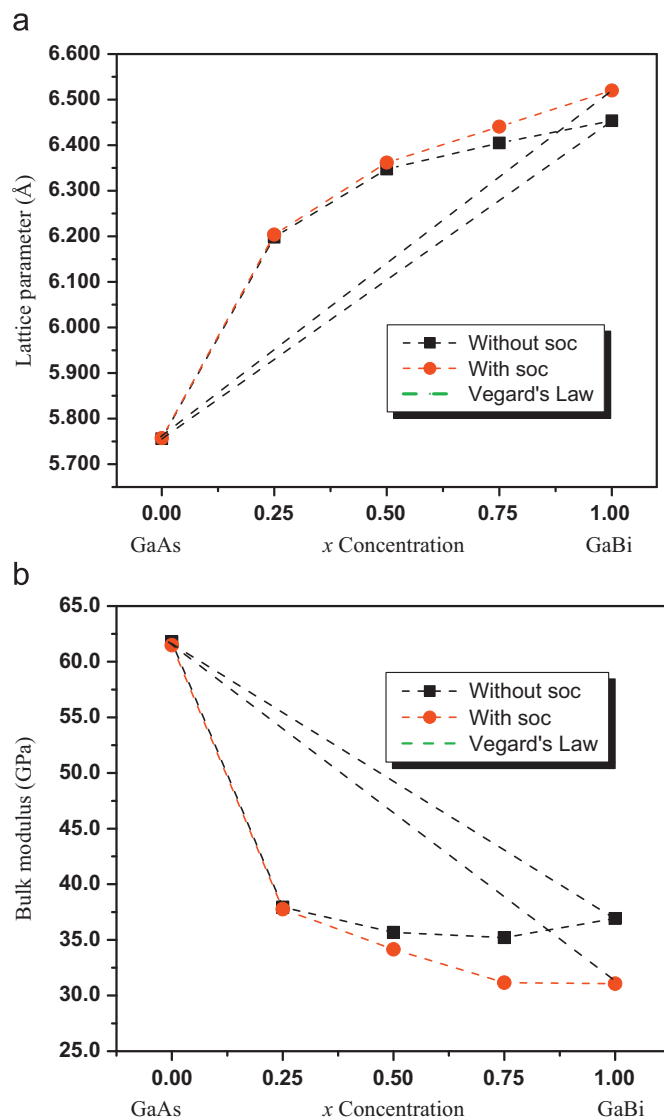


Fig. 2. Variation of calculated lattice parameter and bulk modulus with and without spin-orbit coupling versus Bi concentration in $GaAs_{1-x}Bi_x$ (also comparison with Vegard's law). Calculations are done with GGA.

Table 2

Calculated nearest neighbor bond length distances between Bi–Bi, Ga–Ga, As–As, Ga–As, Ga–Bi and As–Bi in Å for $GaAs_{1-x}Bi_x$ with and without SOC. We have used GGA.

$GaAs_{1-x}Bi_x$	x	Bi–Bi (Å)	Ga–Ga (Å)	As–As (Å)	Ga–As (Å)	Ga–Bi (Å)	As–Bi (Å)
GaAs	0	–	4.06 ^a	4.06 ^a	2.49 ^a	–	–
		–	4.07 ^b	4.07 ^b	2.50 ^b	–	–
$GaAs_{0.75}Bi_{0.25}$	0.25	6.19 ^a	4.86 ^a	4.38 ^a	2.79 ^a	2.38 ^a	4.38 ^a
		6.20 ^b	4.87 ^b	4.39 ^b	2.80 ^b	2.39 ^b	4.39 ^b
$GaAs_{0.5}Bi_{0.5}$	0.5	4.48 ^a	4.95 ^a	4.48 ^a	2.94 ^a	2.57 ^a	4.48 ^a
		4.50 ^b	4.97 ^b	4.50 ^b	2.95 ^b	2.58 ^b	4.50 ^b
$GaAs_{0.25}Bi_{0.75}$	0.75	4.52 ^a	4.12 ^a	6.40 ^a	3.02 ^a	2.70 ^a	4.52 ^a
		4.55 ^b	4.14 ^b	6.44 ^b	3.03 ^b	2.71 ^b	4.55 ^b
GaBi	1	4.56 ^a	4.56 ^a	–	–	2.79 ^a	–
		4.61 ^b	4.61 ^b	–	–	2.82 ^b	–

^a Without spin-orbit coupling.

^b With spin-orbit coupling.

is smaller when SOC is included for both lattice parameter and bulk modulus.

We have also calculated the nearest neighbor bond length distances between Ga, As and Bi with and without SOC. These are given in Table 2. The bond length distances between Ga–As and Ga–Bi are smaller than all other bonds length distances. On applying SOC the bond length distances increase slightly.

In order to study the relation between bond ionicity and total valance charge density, we have calculated the ionicity factor using the empirical formula of Zaoui et al. [18] (apply on only binary compounds):

$$f_i = \left(\frac{S_A}{S_A + \lambda S_C} \right)^\lambda \quad (3.3)$$

where λ is a parameter separating the highly ionic elements from the weakly ionic elements. $\lambda = -1$ for elements and III–V semiconductors; $\lambda = +1$ for II–VI and I–VII semiconductors. Our calculated ionicity factor for GaAs and GaBi is 0.96. Ionicity values close to 1 indicate a covalent nature.

3.2. Electronic properties

3.2.1. Electron charge densities, densities of states and band structures

To explain the bonding properties of $\text{GaAs}_{1-x}\text{Bi}_x$ (at $x=0.0, 0.25, 0.50, 0.75$ and 1.0), we have calculated the electronic charge

density contour in (110) plane with and without SOC. In GaAs, the contour plot shows the clear covalent bonding between Ga and As atoms. SOC does not affect this bonding due to the small electro-negativity difference of Ga (1.81) and As (2.18). Hence in Fig. 3 we show the results for SOC only. At $x=0.25$, the space distribution contour plot shows partial ionic and partial covalent bonding between Ga and As due to As being more electro-negativity than Bi (2.02) and on the other hand Ga–Bi shows stronger covalent bonding due to the small concentration of Bi. SOC does not affect the bonding. At $x=0.50$, the covalent bonding between Ga–As becomes more weak due to increase of Bi concentration whereas it does not affect the bonding between Ga–Bi. But at $x=0.75$, the partial covalent bonding of Ga–As becomes more weak and SOC makes this bonding almost ionic in nature. In binary GaBi, we find a covalent nature. Hence, our calculations show that a high Bi concentration affects the nature of bonding in $\text{GaAs}_{1-x}\text{Bi}_x$ alloys.

To determine the various contributions to the covalent bonding in $\text{GaAs}_{1-x}\text{Bi}_x$ (at $x=0.0, 0.25, 0.50, 0.75$ and 1.0), we have calculated the total density of states (TDOS) and partial density of state (PDOS) for all concentrations (with and without SOC). We show in Fig. 4 the results with SOC only because the results for without SOC are not significantly different. From the PDOS we notice that in GaAs, there is a strong hybridization between Ga-4s² and As-4p³ in the energy range covering –4 up to –6.5 eV. This sp-hybridization causes the strong covalent bonding in GaAs. While As-4s² electrons are localized around –11 eV.

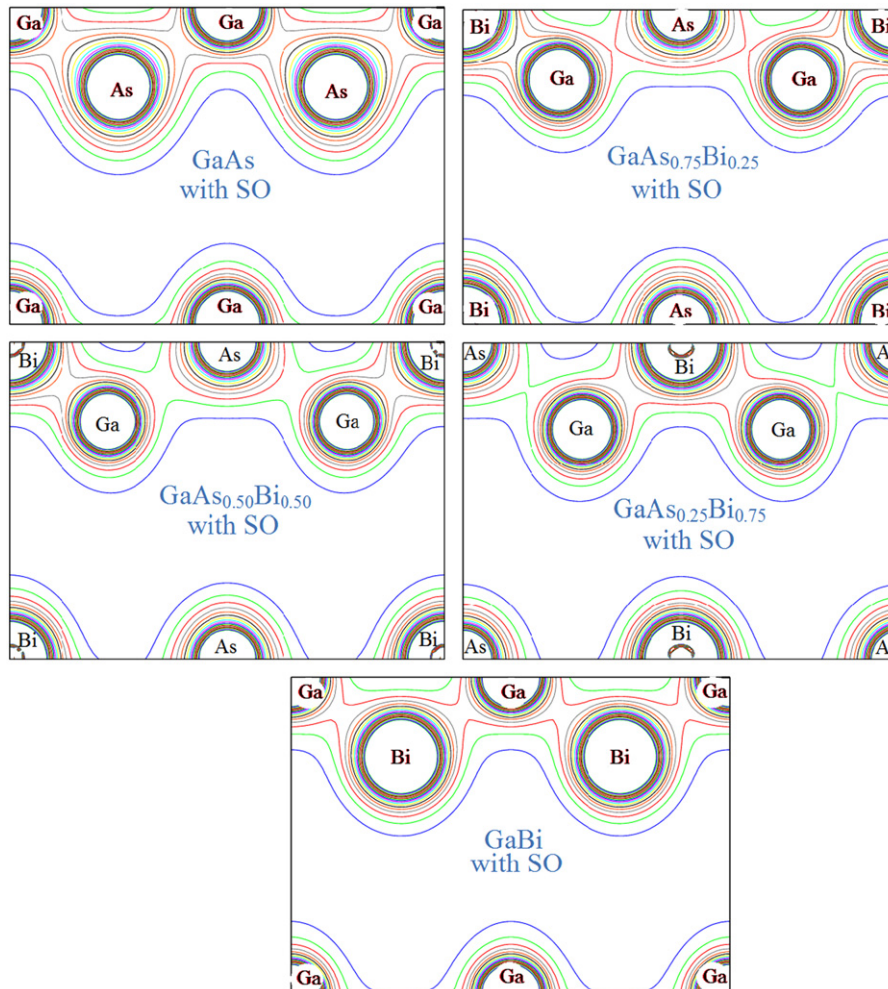


Fig. 3. Calculated space distributed electronic charge density contours in (110) plane with spin-orbit coupling for $\text{GaAs}_{1-x}\text{Bi}_x$ (at $x=0.0, 0.25, 0.50, 0.75$ and 1.0). Calculations are done with GGA.

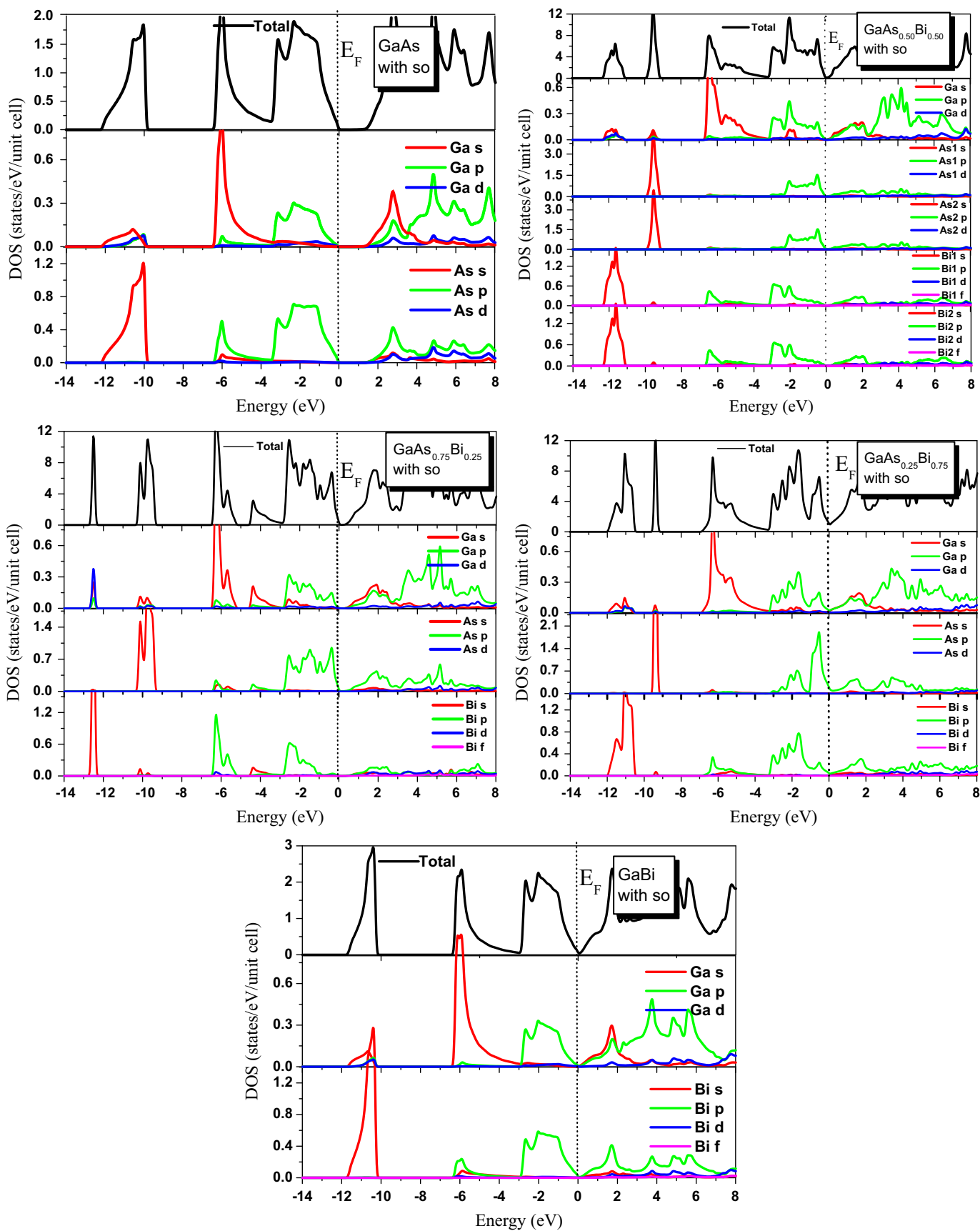


Fig. 4. Calculated TDOS and PDOS with spin-orbit coupling for GaAs_{1-x}Bi_x (at x = 0.0, 0.25, 0.50, 0.75 and 1.0). Calculations are done with GGA.

At Fermi energy level E_F , the p orbitals of Ga and As are dominant and hybridized to form the semiconductor nature. At 25% concentration of Bi, the sp -hybridization becomes small between Ga and As but increases between Ga and Bi resulting in decrease of the covalent bonding between Ga and As. Similar effect was observed with SOC at the same concentration. On increase Bi concentration to 50%, the As- $4p^3$ band at -6.0 eV moves towards the Fermi level and allow Bi- $6p^3$ bands to hybridize with Ga- $4s^2$ band, resulting in a weaker bonding between Ga and As with and without SOC. Also the contribution of As in conduction band is reduced due to increase of Bi content. At $x=0.75$, this sp -hybridization of As with Ga reaches nearly zero, while Ga-Bi sp -hybridization at around -6.0 eV becomes stronger. The As p band near the Fermi level becomes more localized. For GaBi there is strong hybridization between Ga- $4s^2$ and Bi- $6p^3$ around -6.0 eV, while Ga s and p bands hybridize with Bi- p in the energies from the CBM and above.

The calculated band structure of the binary end compounds as well as their alloys indicates a direct band gap located at the gamma point for the whole range of concentrations. Fig. 5(a) shows the electronic band structure for $x=0.0, 0.25, 0.5, 0.75$ and 1.0 using EVGGA and SOC. The effect of SOC is small in the energy scale of the plots. Hence we choose not to show the band structure without SOC. Following Fig. 5 (BS) and Fig. 4 (PDOS) one can see that when we incorporate Bi in GaAs the Bi- $6p$ state, which is located at the valance band maximum (VBM) overlap around the Fermi energy (E_F) resulting in negative band gap; see Table 3. This overlapping is increases with increasing Bi concentration leading to a strong band gap reduction. It was reported that nitrogen in GaNAs perturbs the conduction band and reduces electron mobility [19–21] because nitrogen is highly electronegative (3.04) in addition to its small size, and is attractive to electrons, while in GaAsBi it is expected that Bi perturbs the valence bands and effects the hole mobility [9] because Bi has a low electro-negativity (2.02) in addition to its large size, and tends to be attractive to holes.

The energy band gaps are presented in Table 3. It is clearly seen that the band gap values given by EVGGA are nearest to the experiments and confirm the variation of large energy gap bowing with concentration of Bi. It is clearly seen that the energy gap decreases with increasing Bi concentration. This reduction of the band gap is explained by the highly localized nature of the perturbation introduced by Bi atoms [22–27]. The largest contribution to the band gap reduction originates from structural relaxation and charge exchange that are, respectively, proportional to the differences in the atomic orbital size and energy of the As and Bi atoms [22,25].

We have carefully examined the spin-orbit coupling effect on Bi and As split-off band. In Fig. 5(b), we give a prototype of the low symmetry band structure of the alloys near the Fermi energy to distinguish between Bi- $6p$ heavy holes (HH), Bi- $6p$ light hole (LH) and As/Bi split-off bands. Fig. 6 shows the spin-orbit (SO) split-off (eV) along alloys concentration at 0.25, 0.50 and 0.75, with and without SOC for both As and Bi. It is clearly seen from this figure that SO split-off give bowing in both As and Bi with and without SOC. We calculate the second order quadratic equation to compute the split-off bowing parameter, which are

$$\Delta_0 = -0.48 - 3.44x + 2.24x^2 \text{ As (without SOC)} \quad (a)$$

$$\Delta_0 = -0.72 - 2.28x + 0.64x^2 \text{ As (with SOC)} \quad (b)$$

$$\Delta_0 = -1.51 - 4.48x + 4.48x^2 \text{ Bi (without SOC)} \quad (c)$$

$$\Delta_0 = -1.78 - 3.62x + 3.76x^2 \text{ Bi (with SOC)} \quad (d)$$

where Δ_0 =SO split-off value (eV) and x =Bi concentration.

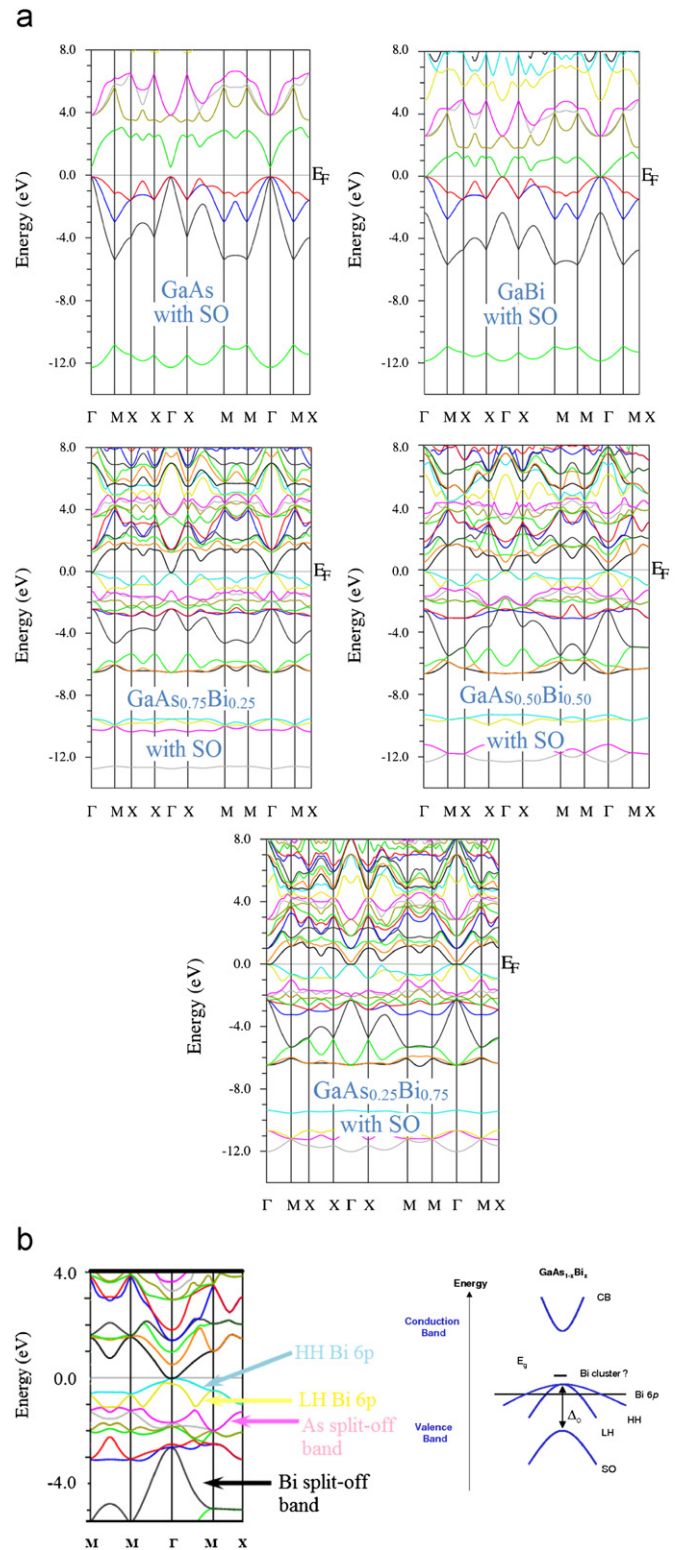


Fig. 5. (a) Calculated band structures with spin-orbit coupling for $\text{GaAs}_{1-x}\text{Bi}_x$ (at $x=0.0, 0.25, 0.50, 0.75$ and 1.0). (b) Close prototype of band diagram for alloys to understand the spin-orbit split-off band variation of As/Bi p band on applying SOC. Calculations are done with EVGGA.

The split-off bowing parameters without SOC for As and Bi are 2.24 and 4.48, respectively. The bowing parameters with SOC for As and Bi are 0.64 and 3.76, respectively. Using SOC, the split-off bowing is reduced drastically for As but a small change in giant bowing of Bi, which is in excellent agreement with results of

Table 3

Comparison of the experimental and theoretical band gap values for $\text{GaAs}_{1-x}\text{Bi}_x$. Our calculations were performed with EVGGA. The theoretical band gap taken from Refs. [2,32] are scissors corrected by adding the difference between the calculated band gap and the measured one. While our results show the actual calculated band gaps without adding the scissors corrections.

X	Band gap energy (eV)		
	Experimental	Theoretical	
		Without SOC	With SOC
$\text{GaAs}_{1-x}\text{Bi}_x$			
0	1.52 ^a	1.51 ^b , 1.52 ^c , 1.20*	0.98*
0.25		0.43 ^c , 0.38*	0.33*
0.50		-0.38 ^c , -0.32*	-0.28*
0.75		-1.05 ^c , -0.98*	-0.89*
1	-1.45 ^a	-1.45 ^{b,c} , -1.38*	-1.30*

^a Ref. [29].

^b Ref. [30].

^c Ref. [2].

* This work using EVGGA.

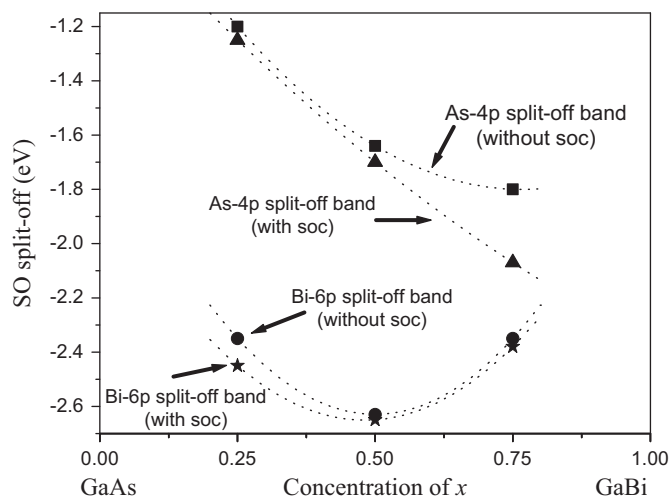


Fig. 6. Bowing effect of spin-orbit split-off band values versus Bi content with and without spin-orbit coupling for $\text{GaAs}_{1-x}\text{Bi}_x$ (at $x=0.25, 0.50$ and 0.75). Calculations are done with GGA.

Bhusal et al. [28]. Bhusal et al. suggested giant bowing in both band gap and split-off values even at low concentration around $x=0.0025$. Our calculated spin-orbit split-off values for binary compounds are 0.30 eV and 2.35 eV for As and Bi, which are in good agreement with 0.34 eV and 2.20 eV reported by Bhusal et al. According to Bhusal et al., these splittings are directly proportional to spin-orbit splitting and inversely proportional to the band gap. The splittings agree well with our values given in Table 3. Hence SOC plays a major role in the large band gap reduction in $\text{GaAs}_{1-x}\text{Bi}_x$.

4. Conclusions

We have presented calculations of structural and electronic properties of $\text{GaAs}_x\text{Bi}_{1-x}$ compounds within the FP-LAPW method. The energy gap, lattice constant, bulk modulus and the SO split-off band are found to vary nonlinearly with Bi concentration. We find that the SOC has a significant effect on the bowing

parameter. The difference in bowing parameters with and without SOC increases with Bi concentration. This is attributed to the fact that SOC for Bi is large compared to Ga and As. Hence on increasing the Bi concentration, we see a bigger effect of SOC. Finally, the densities of states and the band structure are also presented. SOC does not affect the bonding significantly. In agreement with other calculations and experiment, our calculations show that with alloying the valence band (mainly Bi-6p) moves towards the Fermi energy. We find that the binary end compounds and the intermediate concentration alloys show a direct band gaps.

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