

Band structure calculation of the semiconductors and their alloys by Tight Binding Model using SciLab

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Abstract—The tight binding model is one of the strong theoretical techniques to calculate the band gap of the materials. The band structures of some semiconductors and the semiconductors made by their combination is calculated here using simulation technique. The basic theory of Tight Binding Model is presented since beginning to the final matrix formulation. Band structure of the four semiconductors AlAs, AlP, GaAs and GaSb and their corresponding alloys AlAs_xP_{1-x} & GaAs_xSb_{1-x} is computed with the help of TBM formulation using SciLab coding.

Keywords — Tight Binding Model(TBM), Aluminium Phosphide(ALP), Aluminium Arsenide(AlAs), Gallium Arsenide(GaAs) and Gallium Antimonide(GaSb)

I. INTRODUCTION

The band structure of materials does play a very important role for their application purpose. A number of theories and models are there to give the insight of the band structure of the materials. All these models have got their own limitations respond differently to different structures. The materials we will be talking in this report here are semiconductors. The tight binding model is a very strong and interesting approach to solve the electronic band structure[1]. Since the time, it got invented and developed, it has achieved a lot of attention of the researchers all around the world. In solid state physics the band structure calculations are done in the reciprocal space that give rise to real space band picture. The interesting part of the tight binding model is that it picks out band picture of the whole material just by probing at one K point and its nearest neighbours. Well, one can go further, second nearest neighbour and so on, if more accuracy is required in the result. The model has got some limitations also as every model has got. It excludes some interactions and does not take into account every interaction present there in the problem. So, one need to find the interaction parameters of the dominant interaction. The tight binding model has got similarities with the model given by Slater and Koster[2]. Some people do say that the tight binding

model try to join all the threads which were supposed to be broken or incomplete in the model given by Weaire and Thorpe[3], and can be considered the advance version of the Weaire and Thorpe's model[4],[5]. The qualitative and numerical description of the valence band of various materials can be obtained by the tight binding model. Here we are solving band structure of the semiconductors having the diamond or zincblende lattice structures. The interaction parameters are taken from an old reference. The theory is presented in the given report here from very beginning to its final formulation. Well, the matrix formulation shown here does include all the nearest neighbour interactions between s & p orbitals but still there is some error in the electronic energy calculation which occurs at Brillouin zone boundary. The most important part of the simulation done here is that every simulation technique has got its limitations so has the SciLab. And the results may divert from the results obtained from the experiments. Here, the band structure is solved by a computer coding technique, called SciLab. Firstly, the theory is presented in a vary explained manner as possible as it could be. Then, a computer was developed using SciLab and the band structure was computed.

II. BASIC THEORY

The structure of diamond is very well known where each and every carbon atom connected to other carbon atoms with tetrahedral geometrical bonding. The primitive cell of the diamond structure does contain two carbon atoms. The structure of zinc blende also has got the same features. But in zinc blende structure, every atom is not same as it was in the case of diamond structure. The atoms in the diamond or zinc blende structures are sp³ hybridized and this bonding requires an axis set having at least four orbitals in such a way that each atom in the unit cell does possess, one s and three p orbitals. The structure can be solved using tight binding model where nearest neighbour are supposed to be take into the consideration to formulate the matrix which gives band structure. For each tight binding basis function corresponding to every atom, two Bloch functions

are constructed. For a tight-binding basis function $\beta(\mathbf{r})$ we have the two Bloch functions.

$$\Psi_0(\mathbf{k}, \mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} \beta_0(\mathbf{r} - \mathbf{R})$$

&

$$\Psi_0(\mathbf{k}, \mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} \beta_1(\mathbf{r} - \mathbf{R} - \mathbf{y})$$

Where \mathbf{y} is the vector joining the two atoms in the primitive cell and the subscripts on β refer to the

atoms in the primitive cell. In the diamond structure crystals we take $\beta_0(\mathbf{r}) = \beta_1(\mathbf{r})$, but in the zincblende crystals the two functions are different [6]. 8×8 matrix for these normalised basis vectors is given below. The eigenvalue were calculated and plotted in SciLab.

	$\langle s\alpha $	$\langle s\beta $	$\langle p_x\alpha $	$\langle p_y\alpha $	$\langle p_z\alpha $	$\langle p_x\beta $	$\langle p_y\beta $	$\langle p_z\beta $
$\langle s\alpha $	$E(s, \alpha)$	$V(s, s)b_0$	0	0	0	$V(s\alpha, p\mu)$ b_1	$V(s\alpha, p\mu)$ b_2	$V(s\alpha, p\mu)$ b_3
$\langle s\beta $	$V(s, s)b_0^*$	$E(s, \mu)$	- $V(p\alpha, s\mu)$ b_1	- $V(p\alpha, s\mu)$ b_2	- $V(p\alpha, s\mu)$ b_3	0	0	0
$\langle p_x\alpha $	0	- $V(p\alpha, s\mu)$ b_1	$E(p, \alpha)$	0	0	$V(x, x)b_0$	$V(x, y)b_3$	$V(x, y)b_2$
$\langle p_y\alpha $	0	- $V(p\alpha, s\mu)$ b_2	0	$E(p, \alpha)$	0	$V(x, y)b_3$	$V(x, x)b_0$	$V(x, y)b_1$
$\langle p_z\alpha $	0	- $V(p\alpha, s\mu)$ b_3	0	0	$E(p, \alpha)$	$V(x, y)b_2$	$V(x, y)b_1$	$V(x, x)b_0$
$\langle p_x\beta $	$V(s\alpha, p\mu)$ b_1	0	$V(x, x)b_0^*$	$V(x, y)b_3^*$	$V(x, y)b_2^*$	$E(p, \mu)$	0	0
$\langle p_y\beta $	$V(s\alpha, p\mu)$ b_2	0	$V(x, y)b_3^*$	$V(x, x)b_0^*$	$V(x, y)b_1^*$	0	$E(p, \mu)$	0
$\langle p_z\beta $	$V(s\alpha, p\mu)$ b_3	0	$V(x, y)b_2^*$	$V(x, y)b_1^*$	$V(x, x)b_0^*$	0	0	$E(p, \mu)$

Matrix formulated by Tight binding Model

Where ,

$$b_0(\mathbf{k}) = \cos(k_1 a_L/4) \cos(k_2 a_L/4) \cos(k_3 a_L/4) - i \sin(k_1 a_L/4) \sin(k_2 a_L/4) \sin(k_3 a_L/4)$$

$$b_1(\mathbf{k}) = -\cos(k_1 a_L/4) \sin(k_2 a_L/4) \sin(k_3 a_L/4) + i \sin(k_1 a_L/4) \cos(k_2 a_L/4) \cos(k_3 a_L/4)$$

$$b_2(\mathbf{k}) = -\sin(k_1 a_L/4) \cos(k_2 a_L/4) \sin(k_3 a_L/4) + i \cos(k_1 a_L/4) \sin(k_2 a_L/4) \cos(k_3 a_L/4)$$

$$b_3(\mathbf{k}) = -\sin(k_1 a_L/4) \sin(k_2 a_L/4) \cos(k_3 a_L/4) + i \cos(k_1 a_L/4) \sin(k_2 a_L/4) \cos(k_3 a_L/4)$$

$$E(s, \beta) = \langle s\beta | H | s\beta \rangle$$

$$E(p, \beta) = \langle p_x\beta | H | p_x\beta \rangle$$

$$V(s, s) = 4 \langle s\alpha | H | s\mu \rangle$$

$$V(x, x) = 4 \langle p_x\alpha | H | p_x\mu \rangle$$

$$V(x, y) = 4 \langle p_x\alpha | H | p_y\mu \rangle$$

$$V(s\alpha, p\mu) = 4 \langle s\alpha | H | p_x\mu \rangle$$

$$V(p\alpha, s\mu) = 4 \langle p_x\alpha | H | s\mu \rangle$$

The index α stands for anion and the index μ stands for cation.

All the parameters are calculated from following relations [7].

$$V(s, s) = (1/2) \{ [E(\Gamma_1^{\beta}) - E(\Gamma_1^{\nu})]^2 - [E(s, \beta) - E(s, \alpha)]^2 \}^{1/2}$$

$$V(x, x) = (1/2) \{ [E(\Gamma_{15}^{\beta}) - E(\Gamma_{15}^{\nu})]^2 - [E(p, \beta) - E(p, \alpha)]^2 \}^{1/2}$$

$$V(x, y) = (1/2) \{ [E(\Gamma_{15}^{\beta}) - E(\Gamma_5^{\nu})]^2 - [E(p, \beta) - E(p, \alpha)]^2 \}^{1/2}$$

$$V(s\alpha, p\mu) = (1/2) \{ [E(s, \alpha) + E(p, \beta) - 4E(X_1^{\nu})]^2 - [E(s, \alpha) - E(p, \beta)]^2 \}^{1/2}$$

$$V(p\alpha, s\mu) = (1/2) \{ [E(s, \beta) + E(p, \alpha) - 4E(X_3^{\nu})]^2 - [E(s, \beta) - E(p, \alpha)]^2 \}^{1/2}$$

The sums of diagonal energies are related to the energies.

At Γ point,

$$E(s, \beta) + E(s, \alpha) = E(\Gamma_1^{\beta}) + E(\Gamma_1^{\nu}),$$

$$E(p, \alpha) + E(p, \beta) = E(\Gamma_{15}^{\beta}) - E(\Gamma_{15}^{\nu})$$

The remaining two energies are determined by fixing the differences in diagonal matrix elements [7].

$$M_1 = E(1, \beta) - E(1, \alpha) = C_1 (E(s, \beta) + E(s, \alpha))$$

III.SEMICONDUCTORS AND THEIR COMPOUNDS

The band structures of some semiconductors and the compounds made by their combinations have been studied here using TBM and SciLab.

A. Aluminium Phosphide(AIP) and Aluminium Arsenide(AIAs)

The band structure of semiconductors AIAs&AIP and their alloys semiconductor is solved here using the formulation presented above in the theory section. Aluminium arsenide(AIAs) is a III-V compound semiconducting material. The material has got an application in fabrication of the optoelectronic devices like light emitting diodes etc. The structure of Aluminium arsenide (AIAs) is zincblende with a lattice constant having value 5.6605 Å at 300 K. Some other compounds having similar doping configuration are also used for the same purpose. Some of them are gallium arsenide, gallium phosphide. But the application of aluminium arsenide has got its limitations. These limitations in the application of aluminium arsenide are due to inefficiency in the synthesis of pure material. The impurities do help in grain formation and the single crystal formation does not occur. The other important factor which creates limitations in the application is the reactivity of aluminium and the instability of crystals toward the exposure of moisture. AIP crystals also have got zincblende crystal structure with a lattice constant having value 5.451 Å at 300 K. **Aluminium phosphide (AIP)** is a wideband gap semiconductor. This material has got no colour due to the presence of impurities arising from hydrolysis and oxidation.

Here,

$$C_1 = 0.8 \text{ for s orbital}$$

$$= 0.6 \text{ for p orbital}$$

And

$$w = -10.7011 \text{ eV for Al (s orbital)}$$

$$= -5.71060 \text{ eV for Al (p orbital)}$$

$$= -18.6500 \text{ eV for As(s orbital)}$$

$$= -10.0490 \text{ eV for As(p orbital)}$$

$$= -18.9425 \text{ eV for P (s orbital)}$$

$$= -10.6544 \text{ eV for P (p orbital)}[9]$$

Material (a): AIAs[10],[11]

Crystal Structure Zinc Blende
Lattice constant 5.6605 Å
Dielectric constant 10.9

K points	Energy values (eV)[7]
Γ_1^v	-11.73
Γ_1^c	3.04
X_1^v	-9.52
Γ_{15}^c	4.57
X_1^c	2.30
X_3^v	-5.69
X_3^c	2.68
X_5^v	-2.2

Material (b): AIP[10],[11]

Crystal Structure Zinc Blende
Lattice constant 5.4510 Å
Dielectric constant 9.8

K points	Energy values (eV)[7]
Γ_1^v	-12.70
Γ_1^c	3.6
X_1^v	-9.80
Γ_{15}^c	5.6
X_1^c	2.5
X_3^v	-5.4
X_3^c	3.0
X_5^v	-2.26

Here the results obtained from the simulation are shown in graphs presented from fig.1(a) to fig.1(k), in X-axis,

100-200 = gamma point to 'X' point

200-300 = 'X' point to 'K' point

300-400 = 'K' point to 'gamma' point

100-0 = 'gamma' point to 'L' point

Y axis is always indicating Energy in electron-volt.

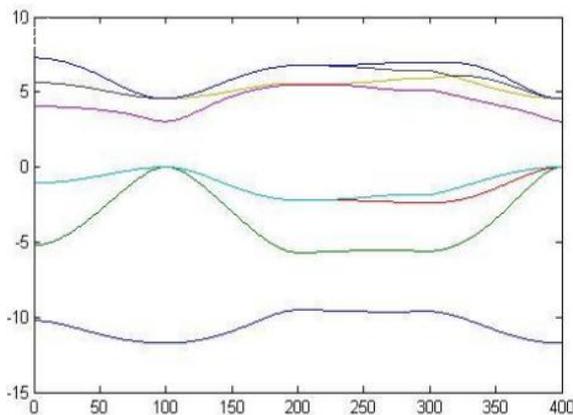


Fig.1(a) Band structure of AIAs($AlAs_x=1, P_{1-x}=0$)

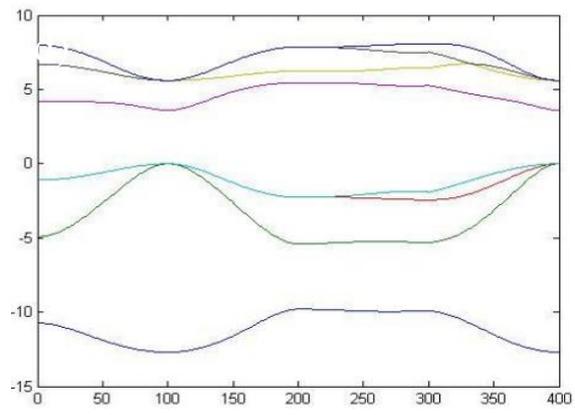


Fig.1(b) Band structure of AIP($AlAs_x=0, P_{1-x}=1$)

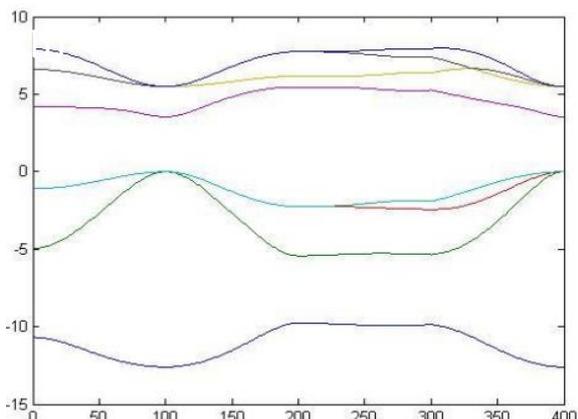


Fig.1(c) Band structure of $\text{AlAs}_{x=0.1}\text{P}_{1-x=0.9}$

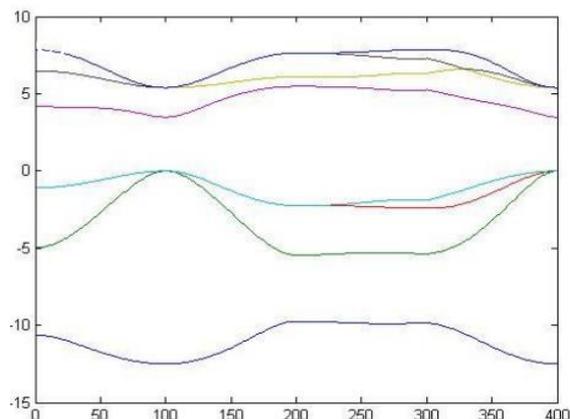


Fig.1(d) Band structure of $\text{AlAs}_{x=0.2}\text{P}_{1-x=0.8}$

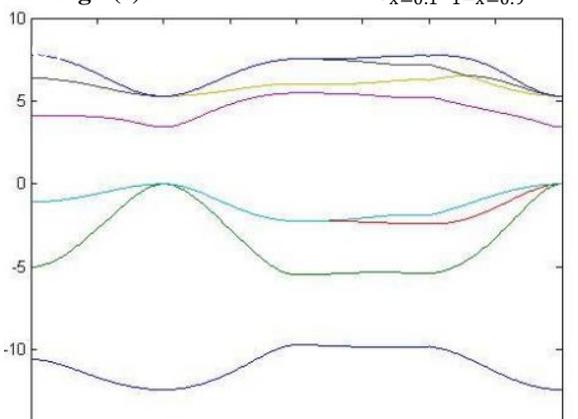


Fig.1(e) Band structure of $\text{AlAs}_{x=0.3}\text{P}_{1-x=0.7}$

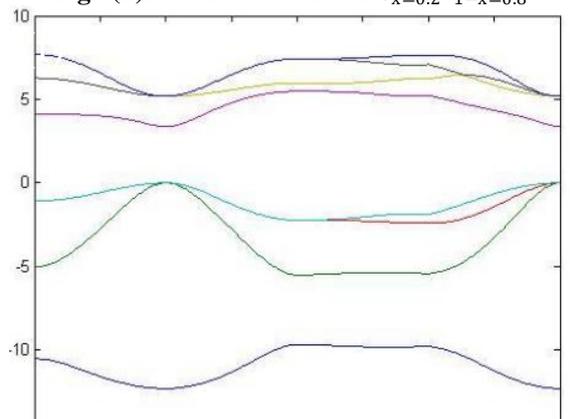


Fig.1(f) Band structure of $\text{AlAs}_{x=0.4}\text{P}_{1-x=0.6}$

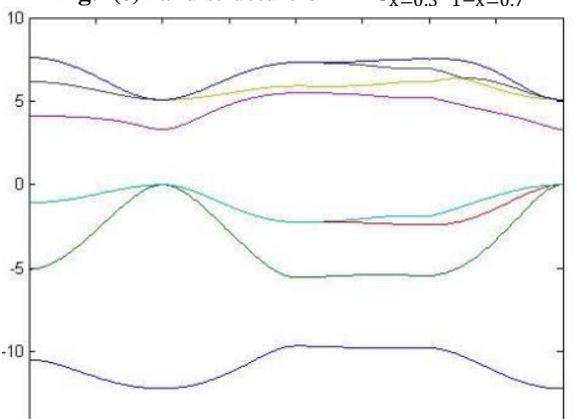


Fig.1(g) Band structure of $\text{AlAs}_{x=0.5}\text{P}_{1-x=0.5}$

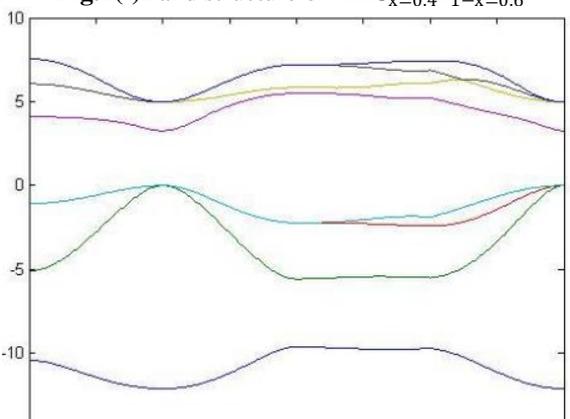


Fig.1(h) Band structure of $\text{AlAs}_{x=0.6}\text{P}_{1-x=0.4}$

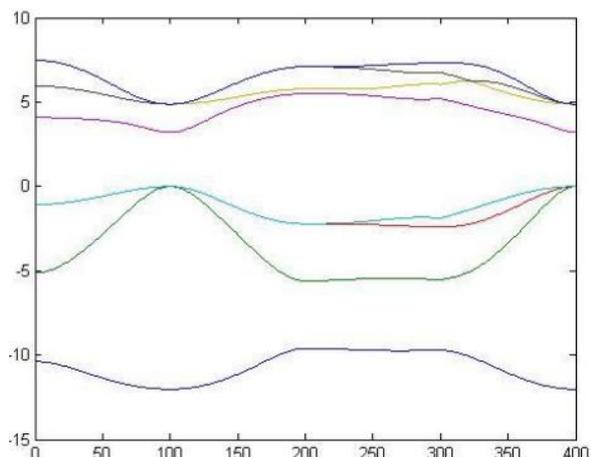


Fig.1(i) Band structure of $AlAs_xP_{1-x}$ with $x=0.7$

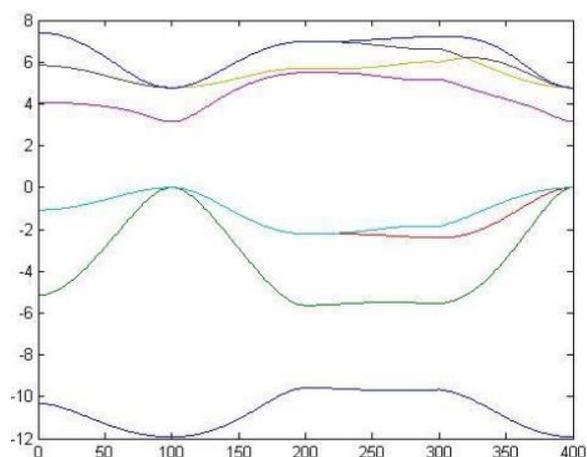


Fig.1(j) Band structure of $AlAs_xP_{1-x}$ with $x=0.8$

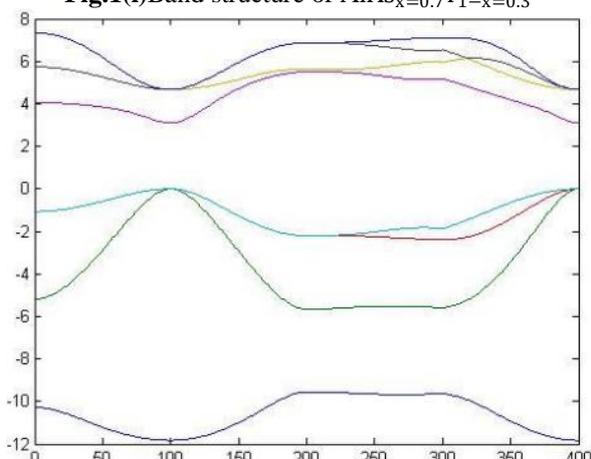


Fig.1(k) Band structure of $AlAs_xP_{1-x}$ with $x=0.9$

Fig. 1 Band structure graphs of Aluminium Phosphide (AlP) and Aluminium Arsenide (AlAs) alloy, obtained from SciLab coding for different proportions of the phosphorus and arsenic, covering whole spectrum of change of the semiconductor from Aluminium Phosphide (AlP) to Aluminium Arsenide (AlAs) with changing mole fraction of the both the semiconductors.

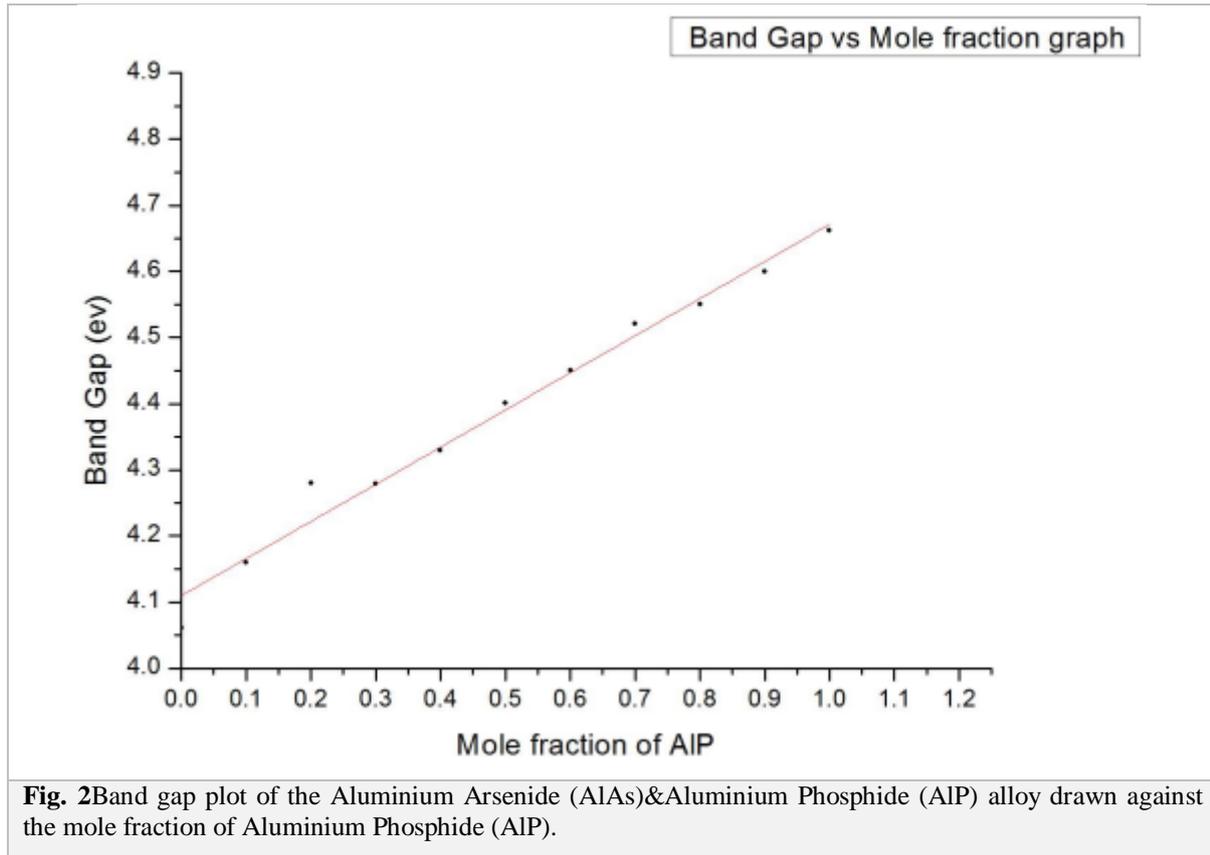


Fig. 2 Band gap plot of the Aluminium Arsenide (AlAs)&Aluminium Phosphide (AlP) alloy drawn against the mole fraction of Aluminium Phosphide (AlP).

B. Gallium Arsenide(GaAs) and GalliumAntimonide(GaSb)

The semiconductors GaAs and GaSb do share the same group. Both are III-V group direct bandgap semiconductors. Both of them do have zinc blende structure. The mobility of charge carriers is higher in GaAs than that of in silicon and germanium. The high mobility is responsible for fast response of the electronic devices made by these semiconductors. The lattice constant of GaAs is similar to that of germanium which helps in the easy fabrication and growth of the GaAs onto the germanium surface. The material (GaAs)has got a lot application for technology part covering from mobile phones to satellite communications and radar systems of high frequencies. It is also used for the fabrication of Gun diodes for microwaves generation.This wide applicability of these materials are enough to attracted one to solve their band structure.

Where $C_1 = 0.8$ for s orbital
 $= 0.6$ for p orbital

And

- $w = 11.549$ eV for Ga s orbital
- $= 5.6712$ eV for Ga p orbital
- $= 18.65$ eV for As s orbital
- $= 10.049$ eV for As p orbital
- $= 15.82$ eV for Sb s orbital
- $= 9.1$ eV for Sb p orbital

Material (a) : GaAs[10],[11]

Crystal Structure Zinc Blende

Lattice constant 5.65325 Å

Dielectric constant 12.9

K points	Energy values (eV)[7]
Γ_1^v	-12.55
Γ_1^c	1.55
X_1^v	-9.83
Γ_{15}^c	4.71
X_1^c	2.03
X_3^v	-6.88
X_3^c	2.38
X_5^v	-2.89

Material (b) : GaSb[10],[11]

Crystal Structure Zinc Blende

Lattice constant 6.09593 Å

Dielectric constant 15.7

K points	Energy values (eV)[7]
Γ_1^v	-12.00
Γ_1^c	0.78
X_1^v	-9.33
Γ_{15}^c	3.77
X_1^c	1.21
X_3^v	-6.76
X_3^c	1.28
X_5^v	-2.37

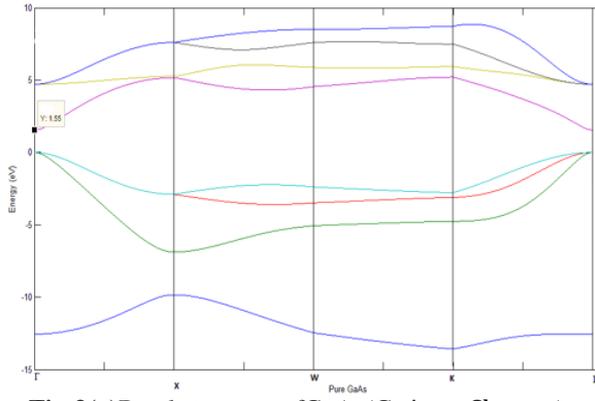


Fig.3(a) Band structure of GaAs ($\text{GaAs}_x=1, \text{Sb}_{1-x}=0$)

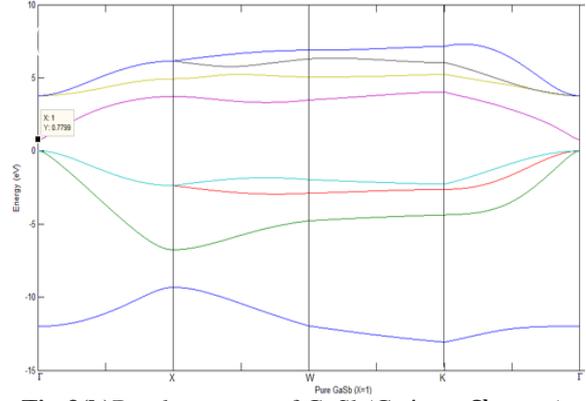


Fig.3(b) Band structure of GaSb ($\text{GaAs}_x=0, \text{Sb}_{1-x}=1$)

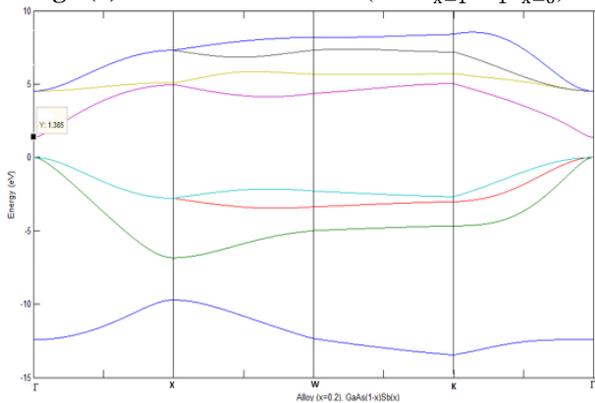


Fig.3(c) Band structure of $\text{GaAs}_{x=0.2}\text{Sb}_{1-x=0.8}$

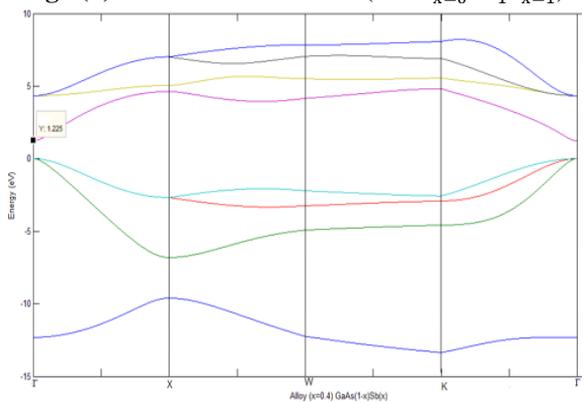


Fig.3(d) Band structure of $\text{GaAs}_{x=0.4}\text{Sb}_{1-x=0.6}$

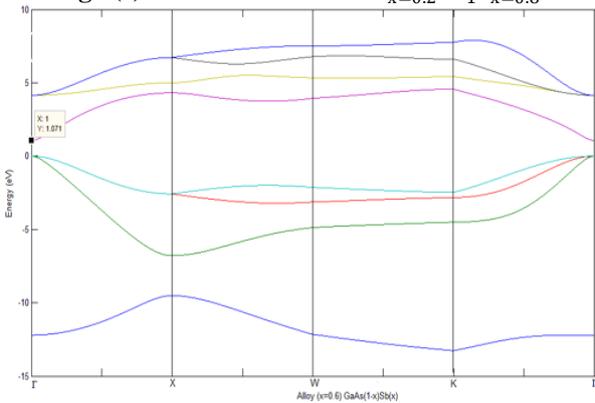


Fig.3(e) Band structure of $\text{GaAs}_{x=0.6}\text{Sb}_{1-x=0.4}$

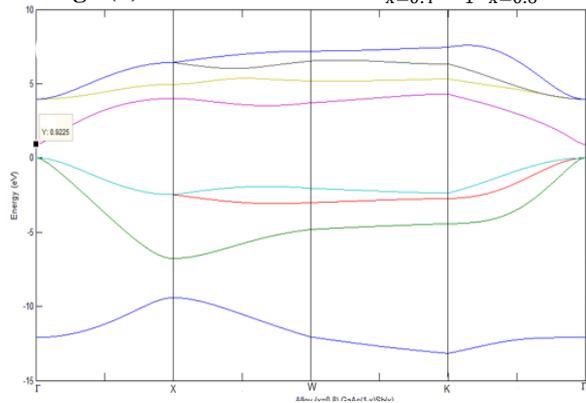
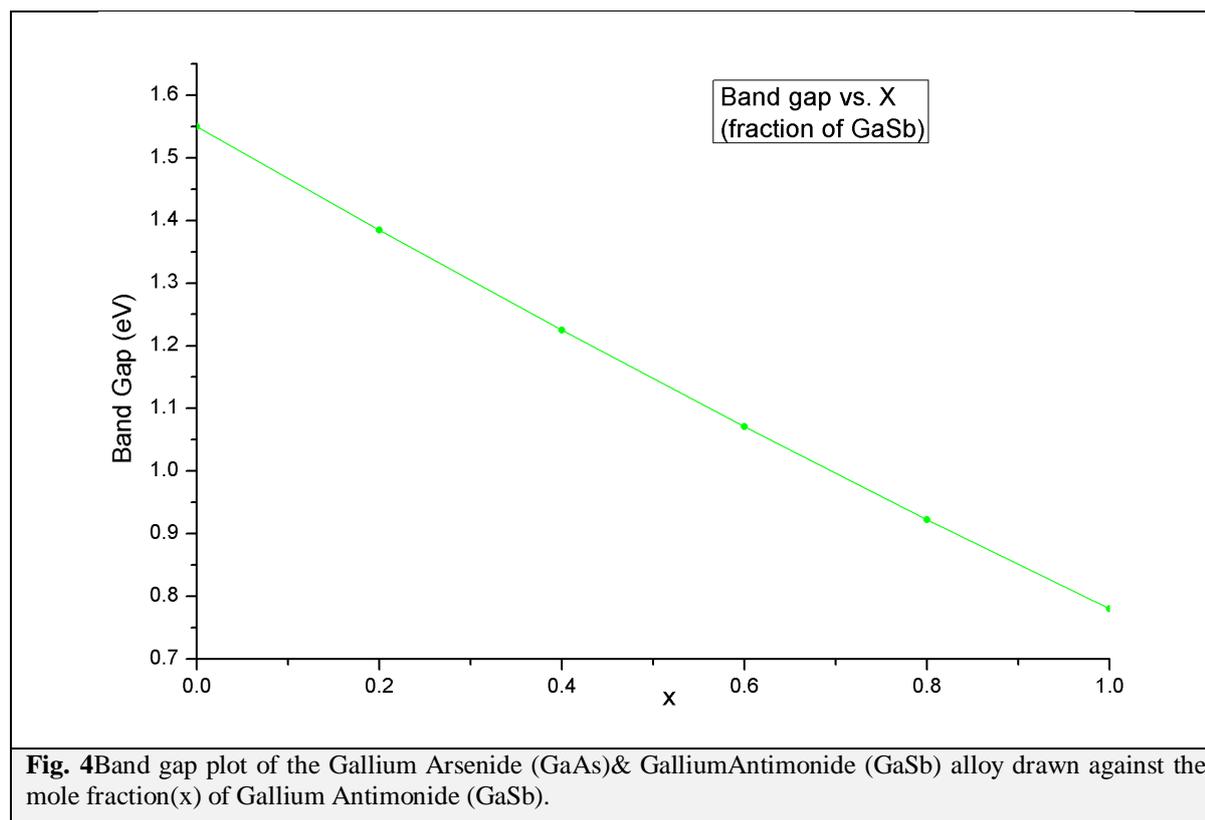


Fig.3(f) Band structure of $\text{GaAs}_{x=0.8}\text{Sb}_{1-x=0.2}$

Fig. 3 Band structure graphs of Gallium Arsenide (GaAs) and Gallium Antimonide (GaSb) alloy, obtained from SciLab coding for different proportions of the antimony and arsenic, covering whole spectrum of change of the semiconductor from Gallium Arsenide (GaAs) to Gallium Antimonide (GaSb) with changing mole fraction of the both the semiconductors.



IV. DISCUSSION

The work presented here does show how the band gap of a compound (alloy) semiconducting material does change against the change in mole fraction of both the participating materials. A linear relationship has been found to occur in the band gap and the mole fraction. As we keep increasing the mole fraction of one of the semiconductor, the band gap of the alloy keeps dominated by that material only. So, these predictions by theoretical computation are of great importance before going for the fabrication of the real semiconducting material having a desired band gap. This computational work does show the relevance and similarities with the predictions reported by other computational techniques.

V. SUMMARY

The band gap calculation, of the alloy semiconductors, is done by a simulating tool, called SciLab. The computer code was developed in SciLab based on the formulation of Tight Binding Model. The tight binding model is one of the strong theoretical techniques to calculate the band gap of the materials. The band structure of semiconductors AlAs, AlP, GaAs and GaSb and their corresponding alloys $\text{AlAs}_x\text{P}_{1-x}$ & $\text{GaAs}_x\text{Sb}_{1-x}$ is computed and presented with nice looking E-k diagrams. The band gap of the alloy semiconductor is plotted against the mole fraction of the original semiconductors. The band gap tuning is found to occur with the mole fraction tuning. A linear relation between the band gap and the mole fraction of the semiconducting material, got

derived from the band structure analysis, obtained from the computation.

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