CALCULATION OF SPIN - RELAXATION TIME OF $Al_xIn_{1-x}Sb$ TERNARY COMPOUNDS USING D' YAKONOV – PEREL MECHANISM

By

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Abstract

This study was designed to investigate the spin – relaxation time of $Al_xIn_{1-x}Sb$ compounds. Spintronic materials (SM) allowed for the exploitation of electron spin to enhance electronic and have huge potential for technological applications. Information is encoded in the spin state of electron of spintronic materials and transferred with the electrons. However, the information is affected by the fact that electron states relaxation is usually characterized by Band – Gap (BG) and Spin – Orbit Splitting (SOS). It thus becomes imperative to understand and have control over spin relaxation in order to retain the information within a required operation period. Equilibrium lattice constants of $Al_xIn_{1-x}Sb$ compounds were determined from Quantum Mechanics (MQ) approach and then compared with the literature results. The results obtained from conduction band effective masses and bulk moduli for the compounds that exhibit SOS were used to determine the spin – relaxation times utilizing D' Yakonov – Perel mechanism. The results showed that the equilibrium lattice constants were 6.3 and 6.1 Å for InSb and AlSb respectively which agreed with literature results of 6.4, 6.1 Å for InSb and AlSb respectively. The SOS of 0.67eV was obtained for all concentrations. Thus, the information encoding ability of $Al_xIn_{1-x}Sb$ decreases with increase in concentration of Aluminum (Al). Moreover, the spin – relaxation time of $Al_xIn_{1-x}Sb$ decreases with increase in Al concentration which makes it a useful material for spintronic applications.

Keywords: Spintronics, D' Yakonov-Perel mechanism, Pseudo-potential, Spin-orbit splitting, Lattice constant.

INTRODUCTION

The goal of electronic structure studies is to be able to calculate physical properties which agree favorably well with experimental data. If this is achieved, confidence is restored in the calculation methods. This confidence allows an identification and detailed interpretation of the microscopic bases of observed phenomena, followed by the prediction of new and unexpected properties and materials. In a situation whereby the work has not been done experimentally, the theoretical prediction can be a starting point for the experimental take–off, i.e. theoretical calculation can be the starting point for the journey to the real expectation.

The growing demand for new technologies stimulates an active research interest in band-gap engineering and phonon dispersion relation of semiconductors. Group III-V materials were chosen because some of these materials crystallize in face-centered cubic structure with direct band-gap which especially constitute the building blocks of emitters in cellular, satellite and fiber glass communication (Lachebi, 2008). Band-gap engineering is a procedure in which quantum physics can be used to simulate the application-based properties of materials. This can be achieved by changing specific attributes such as atomic composition, concentration of impurity or dopant of the materials until the desired properties are obtained, which may give rise to new materials. In computational material sciences, computer programmers make use of variables, experimentally determined parameters as input.

However, nowadays, simulations of solids and molecules are performed using first-principles. One incentive for studies in the field of condensed matter was and still is the study and development of materials for the next generation of computers (Remediakis and Efthmios, 1999). Most electronic devices employed circuits which express data and other information in the form of binary digits. As technology advances, the size of individual semiconductor material approaches the dimension of an atom, thus marking the end of the silicon road map (Sarma and Fabian, 1999). This enhances the multifunctionality of devices, i.e., a device carrying out processing and data storage on the same chip.

LITERATURE REVIEW

Previous studies had established that in a many-electron system, the potential is more complicated because of electron-electron interactions(V_{e-e}) electron-nucleus interaction(V_{e-n}) and perhaps nucleus-nucleus interactions. Thus, the Schrödinger equation for many-electron system is

$$\left(\frac{-\hbar^2}{2n}\nabla^2 + \left(V_{e-e}(r) + V_{e-n}(r) + V_{n-n}(r)\right)\right)\psi(r) = E\psi(r) \quad (1)$$

If equation (1) is solved, parameters useful for electronic and optical technology can be obtained with computational technique (Alexander et al., 2008).

Born-Oppenheimer approximation for system of electrons of mass m, nuclei of mass M at positions r and R, respectively, the non-relativistic Hamiltonian $\widehat{H}$ is written as:

$$H = \sum_i \frac{p_i^2}{2m} - \sum_{j,i} \frac{Z_j e^2}{4\pi \in |r_i - R_j|} + \frac{1}{2}\sum_{i,i'}{}' \frac{e^2}{4\pi \in |r_i - r_{i'}|} + \sum_j \frac{p_j^2}{2M_j} + \frac{1}{2}\sum_{j,j'}{}' \frac{Z_i Z_{j'} e^2}{4\pi \in |R_j - R_{j'}|} \quad (2)$$

In Born-Oppenheimer approximation method, the heavy nuclei are regarded as frozen core because the nuclear motion is negligible relative to electronic motion.

The description of the physical properties of interacting many-particle systems, density functional theory, (DFT) is one of the problems that require solution of a Schrödinger equation with 3N spatial variables and N-spin variables (for electrons). N is the number of particles in the system. For atoms, N ranges from one to 100-electrons and often more than 100electrons. In a solid, N$\sim 10^{23}$(Leenwen, 1994; Kohn, 1999). Therefore it is clear that this problem cannot be solved without some approximation along the line, somewhere.

The main objective of DFT is to understand the properties of many-body particle systems(Gonze, 2007) and calculate several measurable quantities, like bonding energy, polarizability, conductivity, etc. rather than the wave function itself(Harrison, 1980).

Mechanisms of spin relaxation

Elliott-Yafet Mechanism

This mechanism is suitable for elemental semiconductor with symmetry invasion, i. e., and centrosymmetric.

D' Yakonov-Perel Mechanism

D' Yakonov-Perel mechanism is good for calculation of spin-orbit splitting of the conduction band in non-centrosymmetric semiconductors like GaAs (but not Si or Ge, which are centrosymmetric).For bulk semiconductors, this splitting was first pointed out by Dresselhaus (Restrepo and Windl, 2012). In contrast to the Elliott-Yafet mechanism,the spin rotates not during, but between the collisions

Bir–Aronov-Pikus Mechanism

Bir–Aronov-Pikus mechanism is a mechanism of spin relaxation of non-equilibrium electrons in p-type semiconductors due to the exchange interaction between the electron and hole spins (or, expressing it otherwise, exchange interaction between an electron in the conduction band and all the electrons in the valence band (Sarma and Fabian, 1999).

Spin-Relaxation Time

Spin-relaxation and spin-dephasing are processes which lead to spin-equilibrium by bringing an unbalanced population of spin states into equilibrium.

Most of the binary and ternary compounds found in groups (III-V) and groups (II-VI) semiconductors lack inversion symmetry; momentum states of the spin up and spin down electrons are not degenerate, i.e.,$E_{k\uparrow} \neq E_{k\downarrow}$. Inversion symmetry is broken due to the presence of two distinct atoms in the Bravais lattice.

For inversion asymmetry systems, D' Yakonov-Perel mechanism was found suitable for spin-relaxation time calculation.

The Elliott-Yafet relation gives an order-of-magnitude estimate of spin-relaxation time, τ_s by relating it to the shift Δg of the electronic g-factor from the free electron value$g_o = 2.003$ as;

$$\frac{1}{\tau_s} \approx \frac{(\Delta g)^2}{\tau_p} \qquad (3)$$

Where τ_p is the momentum relaxation time and for semiconductors with inversion symmetry,

$$\frac{1}{\tau_s} = A(\frac{\Delta_{so}}{E_g + \Delta_{so}})^2 \left(\frac{E_k}{E_g}\right)^2 \frac{1}{\tau_p} \qquad (4)$$

Using equation (3) in (4),

$$\frac{1}{\tau_s} = A(\frac{\Delta_{so}}{E_g + \Delta_{so}})^2 \left(\frac{E_k}{E_g}\right)^2 \frac{1}{\tau_s(\Delta g)^2} \qquad (5)$$

$E_g$is the energy gap and Δ_{so} is the spin-orbit splitting of the valence band and the numerical factor A is in the order of unity. D' yakonov-Perel mechanism is mostly used for a semiconductor that lacks inversion symmetry such as binary and ternary compounds. Spin-relaxation time can be calculated using (Restrepo and Windl, 2012);

$$\frac{1}{\tau_s(E_k)} = \frac{32}{105}\gamma_3^{-1}\tau_p(E_k)\alpha^2\frac{E_k^3}{\hbar^2 E_g} \qquad (6)$$

Where α determines the strength of the spin-orbit interaction. Lamour frequency vector $\omega(k) = \alpha\hbar^2(2m_c^3E_g)^{-\frac{1}{2}}$ (7)

Expressions for α and $\tau_p$can be obtained in eqs. (3 and 6). Thus equation (7) becomes;

$$\frac{1}{\tau_s(E_k)} = \frac{32}{105}\gamma_3^{-1}(\Delta g)^2\tau_s(E_k)\left(\frac{\omega(k)}{\hbar^2(2m_c^3E_g)^{-1/2}}\right)^2\frac{E_k^3}{\hbar^2 E_g} \qquad (8)$$

Equation (8) describes spin-orbit splitting (spin-dephasing) in bulk III-V semiconductors. Phonon frequency, $\omega(k)$ can be obtained from phonon dispersion relation while energy gap, E_g obtained from the band structure of the semiconductor material.

For impurity scattering, $\gamma_3 = 6$; for acoustic phonons, $\gamma_3 = 1$; and for optical polar phonons, $\gamma_3 = {}^{41}/_{6}$.

Neither electron-phonon nor phonon dispersion relation for InAlSb ternary compounds could not be obtained due to incapability of the available software and constant power source to sustain the calculations. However relaxation time has been calculated using equation (Pil Hun and Kim, 2001):

$$\frac{1}{\tau_s} = Q\alpha^2 \frac{(k_B T)^3}{\hbar^2 E_g} \tau_p \qquad (9)$$

When $E_k = k_B T$ and $Q = \frac{32}{105}\gamma_3^{-1}$ for impurity scattering, eq. (8) is equivalent to eq. (9) and momentum-relaxation time,τ_p, is;

$$\tau_p = \frac{8\sqrt{\pi}}{3} \frac{\hbar \mathcal{R}^{\frac{3}{2}}}{E_1^2 (k_B T)^{\frac{3}{2}}} \left(\frac{m_0}{m_c}\right)^{\frac{3}{2}} a_0^3 c_l \qquad (9a)$$

$$m_c^* = \frac{m_c}{m_o} = \frac{1}{1 + \frac{2P^2}{3m_o}\left(\frac{2}{E_g} + \frac{1}{E_g + \Delta_{so}}\right)} \qquad (9b)$$

Where, $P = \frac{h}{a_o}$.

For impurity scattering, $\gamma_3 = 6$ and $\frac{32}{105}\gamma_3^{-1} = 1.83$. But Q varies from 0.8 to 2.7. Thus Q value of 1.75 ($\frac{0.8+2.7}{2}$) will be used in this research.

The longitudinal elastic constant is

$$c_l = \frac{3c_{11} + 2c_{12} + 3c_{44}}{5} \qquad (10)$$

The three independent elastic constants for cubic lattice are$c_{11},\ c_{12}\ and\ c_{44}$. They are related to the isotropic bulk modulus B, resistance to shear deformation C, and shear modulus G, respectively (Mattesini et al., 2009) as

$$B = \frac{1}{3}(c_{11} + 2c_{12}) \qquad (10a)$$

$$C = c_{44,} \qquad (10b)$$

G= $\frac{1}{2}(c_{11} - c_{12})$ $(10c)$

In an isotropic solid (Bardeen and Shockley, 1950; Marqueset al., 2003)

$c_{44} = \frac{1}{2}(c_{11} - c_{12})$. (11).

For a complete isotropic material,

$$C = G \quad (12)$$

Also, Cauchy relations

$$c_{11} = 3c_{12} \quad (12a)$$

$$c_{44} = c_{12} \quad (12b)$$

are valid for isotropic cubic crystals (Bardekn and Shockley, 1950)

Thus eq. (10a) becomes

$$B = \frac{1}{3}(3c_{12} + 2c_{12}) \quad (12c)$$

Thus, $c_{12} = \frac{3B}{5}$ and $c_{44} = \frac{1}{2}\left(c_{11} - \frac{c_{11}}{3}\right) = \frac{c_{11}}{3}$

That is$c_{11} = 3c_{44} = 3c_{12}$

Thus, $c_{44} = c_{12} = \frac{3B}{5}$ $(12d)$

$$c_{11} = \frac{9B}{5} \quad (12e)$$

Effective mass,$m_c^* = \frac{m_c}{m_0} = \frac{1}{1+\frac{2P^2}{3m_0}\left(\frac{2}{E_g}+\frac{1}{E_g+\Delta_{so}}\right)}$ (13)

$$\alpha = \frac{4\eta}{\sqrt{3} - \eta}\frac{m_c}{m_0} \quad (13a)$$

$$\eta = \frac{\Delta_{so}}{E_g + \Delta_{so}} \quad (13b)$$

Deformation potential energy, $E_1 = a_0 \left[\frac{E_c(a_0+\Delta a_0)-E_c(a_0-\Delta a_0)}{2\Delta a_0}\right]$ (20)

Room temperature: $T = 300K$, Ryberg constant, $\mathcal{R} = 2.17991x10^{-18}J$, Plank's constant, $\hbar = 1.05459x10^{-34}Js$ and Boltzmann constant, $k_B = 1.381x10^{-23}J/K$.

Electronic spin-relaxation times for silicon, diamond and graphite semiconductors were calculated using the Elliott-Yafet mechanism (Restrepo and W.Windl, 2012).

Spin relaxation time of conduction electrons through the Elliot-Yafet, D'yakonov-Perel and Bir-Aronov-Pikus mechanisms were calculated theoretically for bulk GaAs, GaSb, InAs and InSb of both n- and p-type (Pil Hun and Kim, 2001). Also, theory of spin relaxation of conduction electrons was reported by Sarma and Fabian (1999).

In electronics, integrated circuits operate by controlling the flow of carriers through the semiconductor by the applied electric field. These integrated circuits function as high signal processing devices but the processed information is lost immediately the power is switched off because the information is stored as charges in capacitors (Hong et al., 2004; Dederichs et al., 2005). Nowadays, new devices generally called spintronics exploit the ability of conduction electrons in metals and semiconductors to carry spin-polarized current. Spintronics, or spin electronics, involves the study of active control and manipulation of spin degrees of freedom in solid-state systems. Spin transport differs from charge transport in that spin is a non-conserved quantity in solids due to spin-orbit and hyperfine coupling.

Another potentially significant property of spin is its long coherence or relaxation time, i.e. it tends to stay that way once it is created. One of the key obstacles to spintronic device operation and spin-based quantum information processing is the spin relaxation and spin dephasing (the decay of the longitudinal and transverse spin components) respectively. Spin relaxation and spin dephasing, in principle, also originate from the spin interactions; the fluctuation or in-homogeneity in spin interactions leading to spin relaxation and spin dephasing (Sarma and Fabian, 1999).

RESEARCH METHODOLOGY

Quantum Espresso-5.4.0 version was downloaded and installed to process $Al_x\mathrm{In}_{1-x}\mathrm{Sb}$ ternary compounds. Experimental lattice constants and atomic masses of the binary compounds were obtained from electronic sources, journals and textbooks. The pseudo-potentials used were downloaded from the Quantum Espresso website. One of the objectives of this work is to assess the influence of pseudo-potentials on the studied properties. First-principles total energy calculations were performed within the frame work of Density Functional Theory (Giannozzi et al., 2009). Equilibrium lattice constants, a_o, bulk modulus B_o and pressure derivatives,B_o', of the bulk modulus for each compound were calculated using the standard procedure by fitting total energy against volume to a Murnaghan's equation of states (Marques et al., 2003). These stable parameters were inserted into the self-consistence field input codes as embedded in the Quantum Espresso software package for calculating the total energy and Fermi energy for the system. Since convergence with respect to energy cutoff is a property of pseudo potentials, it was carefully performed for each compound up to the energy difference of $10^{-3}Ry$ for hard pseudo-potentials.

Results

Due to the fact that energy-gap of InSb was the lowest, followed by that AlSb, Al was used as dopant in $Al_xIn_{1-x}Sb$ ternary compounds. Tables of results are follows:

Table 1. Comparison of Energy-GapsE_g, lattice constants,a_o, of InSb and AlSb binary compounds

Compounds	Lattice Const $\boldsymbol{a_o}$ **(a.u)**		Energy gap (eV)
InSb	6.298	6.4788[10]	0.63
AlSb	6.111	6.1355[10]	1.25

[10]Papis-Polakowska, (2006)

Table: 2. Calculated lattice constant, a_o, bulk modulus, B_o and pressure derivatives B_0^1 for $Al_xIn_{1-x}Sb$ Ternary Compounds.

Concentration, x	a_o(a.u)	B_o (GPa)	B_0^1
0.00	11.90	210.50	4.66
0.25	11.80	213.80	4.25
0.50	11.71	216.80	3.61
0.75	11.62	220.40	4.93
1.00	11.52	222.20	4.18

Table: 3. Calculated Energy-Gap (E_g), Spin-Orbit Splitting(Δ_o)and Spin-relaxation time (sec) for $Al_xIn_{1-x}Sb$ using PAW-PP with SOC

Concentration, x	E_g (eV)	Δ_o (eV)	τ_s (sec)
0.00	0.17	0.67	0.11
0.25	0.37	0.67	0.049
0.50	0.80	0.67	0.029
0.75	0.93	0.67	0.027
1.00	1.00	0.67	0.025

Discussions

Structural Parameters

Lattice constants calculated for the $Al_xIn_{1-x}Sb$ ternary compounds decreased with increasing concentrations of Al. This was expected because lattice constant of InSb is greater than that of AlSb binary compounds. In $Al_xIn_{1-x}Sb$, energy-gap increases with increasing concentration but, lattice constant decreases with increasing energy-gap in $Al_xIn_{1-x}Sb$. Result revealed also that Spin-relaxation time calculated for $Al_xIn_{1-x}Sb$ ternary compound (with SOC) decreases with increasing Al concentration. Finally, optical frequency decreases in $Al_xIn_{1-x}Sb$ with increasing concentration from 0.25 to 0.75.

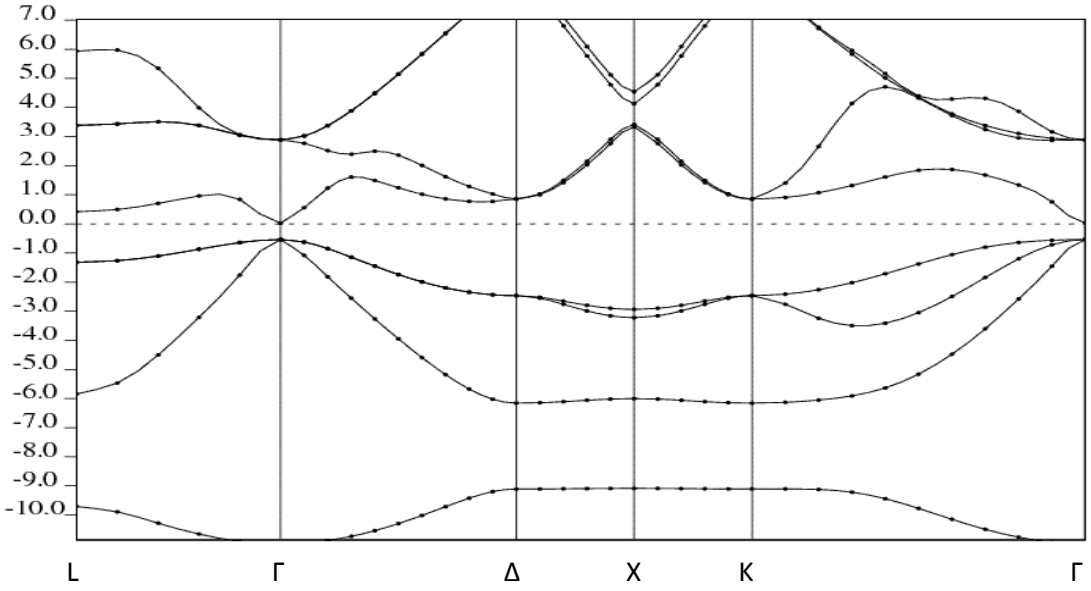

Fig. 1. Band structure of Indium Antimonide (GGA)

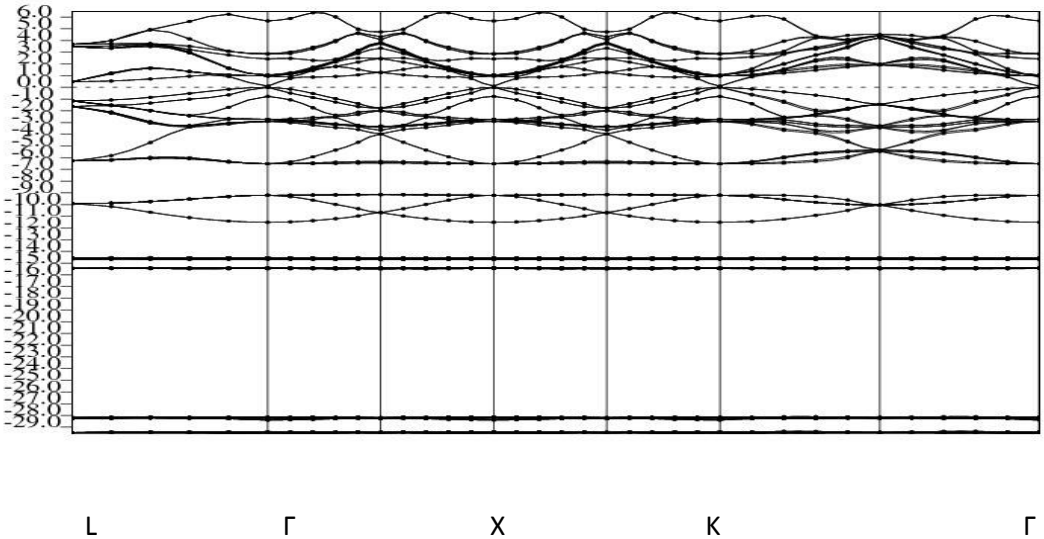

Fig. 1a. $Al_{0.0}In_{1.0}Sb$

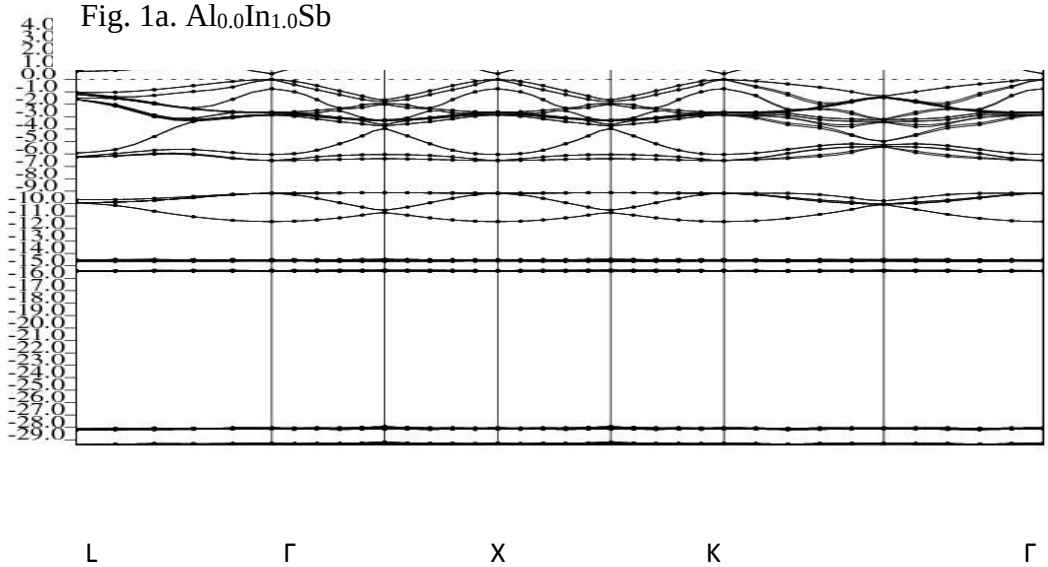

Fig. 1b $Al_{0.25}In_{0.75}Sb$

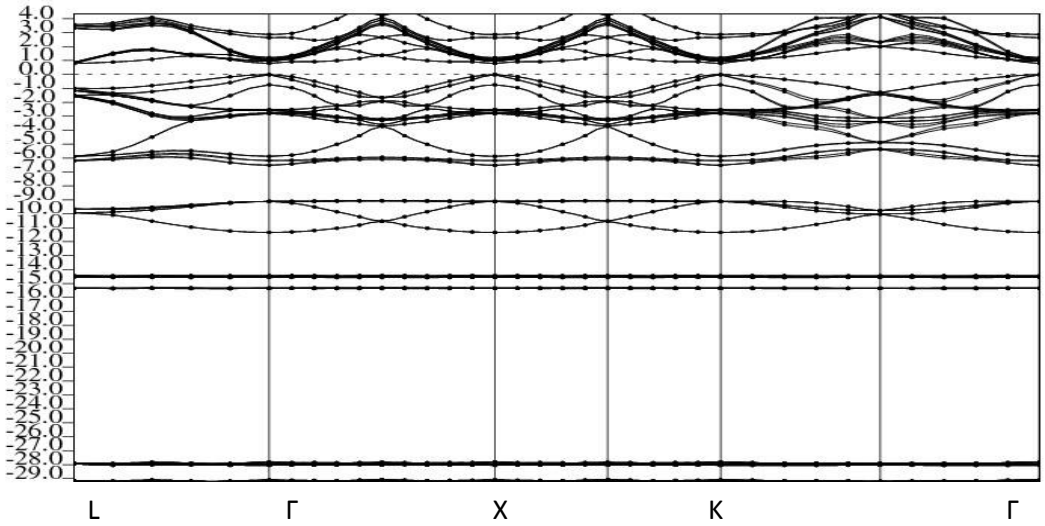

Fig. 1c. $Al_{0.5}In_{0.5}Sb$

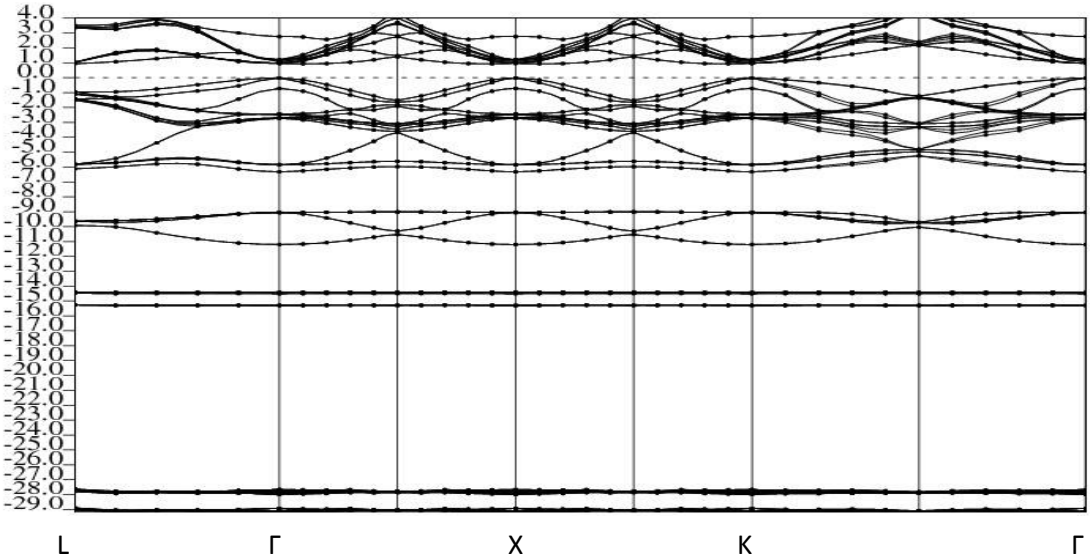

Fig. 1d. $Al_{0.75}In_{0.25}Sb$

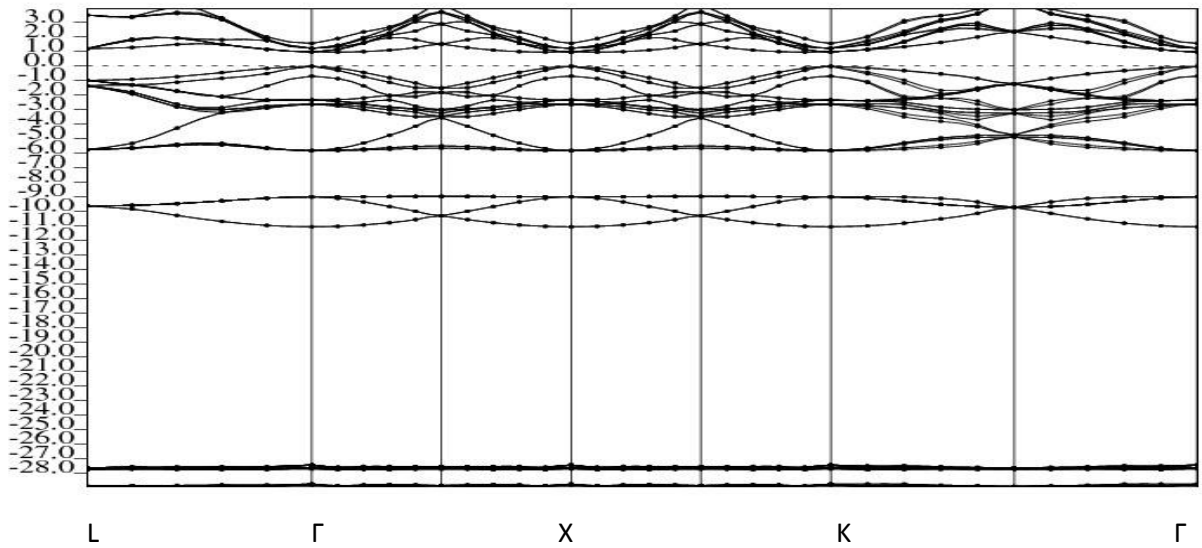

Fig.1e. $Al_{1.0}In_{0.0}Sb$

Conclusions

In conclusion, spin relaxation times calculated for $Al_xIn_{1-x}Sb$ decreases with increasing concentration. Thus the shortest time for information transfer can be obtained at higher concentration of Al (Pil Hun and Kim, 2001).

It can also be inferred that, modern electronic structure techniques such as Quantum Espresso can produce fine details, especially for phonon spectra of semiconductors. This gives further confidence in the predictive power of these techniques.

The results equally showed that UV-wavelength range for the $Al_xIn_{1-x}Sb$ is 364.5–253.1 nm.

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