

Investigation of Transport Properties of $\text{InP}_{1-x}\text{Sb}_x$ alloys: A First Principle Approach

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Abstract: The transport properties of $\text{InP}_{1-x}\text{Sb}_x$ supercell structures have been analyzed at different percent of Sb incorporation. The investigation has been performed employing the BoltzTraP code, which emphasizes on parameters computed using WIEN2K package under Density Functional Theory (DFT) formalism. The transport parameters calculation assumes constant value of relaxation time. The analysis of such parameters as a function of temperature predicts: (a) the distribution of carriers along different bands (i.e., both valence and conduction band); (b) the type of degeneracy of the material; (c) the electrical conductivity and mobility of the alloy.

Keywords: III-V semiconductor; BoltzTraP Code; Transport Property; Hall Coefficient.

1. Introduction

During the last few decades, InP has been a potential substrate for various electronic and optoelectronic devices applications¹⁻⁸. This is primarily due to the consequence of high mobility in InP compounds⁹. Occurrence of such significant properties has encouraged various research groups to perform intensive studies (both, theoretical and experimental) on various InP related alloys¹⁰.

$\text{InP}_{1-x}\text{Sb}_x$ has been reported to have direct band gap along Sb composition range with significant amount of band gap bowing^{9,11}. In $\text{P}_{1-x}\text{Sb}_x$ is grown employing various epitaxial techniques¹³⁻¹⁷. The material undergoes a higher degree of super-saturation due to its large miscibility gap and is also meta-stable in nature^{13,14}. The empirical¹⁸ and computational

^{11,12,9} studies performed analyzes on the structural, electronic and thermodynamic properties of $\text{InP}_{1-x}\text{Sb}_x$ alloy, at various percentage of Sb incorporation. The investigation of such properties asserts the material to be thermodynamically stable⁹.

The contradictory phenomenon of enhancement in spin-orbit splitting energy with reduction in band gap, at increased Sb incorporation, leads to lowering of Inter Valence Band Absorption (IVBA) effects. Hence, proclaiming the competency of $\text{InP}_{1-x}\text{Sb}_x$ alloy for optoelectronic applications. Moreover, a significant reduction in effective mass parameter for CB (Conduction Band) as compared to the Valence Sub-bands, confirms the contribution of the conduction band electrons to the transport properties of the material¹¹. This phenomenon urges to further investigate the transport properties of $\text{InP}_{1-x}\text{Sb}_x$ alloy, at various percentage of Sb incorporation.

This paper reports for the first time to my knowledge, a detailed insight into the transport properties of $\text{InP}_{1-x}\text{Sb}_x$ supercell structure at different percentage of Sb incorporation. The transport parameters have been computed employing the BoltzTraP Code¹⁹ (in association with WIEN2K package²⁰), considering constant relaxation time approximation.

2. Computational Methods

The computation for obtaining necessary parameters has been implemented using the Full Potential Linear Augmented Plane Wave (FP-LAPW) method based on Density Functional Theory (DFT) formalism, employing WIEN2K package²⁰. It utilizes the PBE-GGA²¹ and TB-mBJ²² scheme for calculation of the exchange-correlation potential and exchange potential, respectively. The valence states of In, P and Sb are $4d^{10}5s^25p^1$, $3s^23p^3$ and $4d^{10}5s^25p^3$, respectively. The basis sets comprising s, p and d orbitals have been used for both cation and anion atoms for all the structures. A multiplicity of $1 \times 1 \times 1$ of the elementary InP supercell leads to the formation of 8 atoms supercell structure. A mesh consisting of 50 k points has been considered in the irreducible wedge of the Brillouin zone. Bulk InP has a Zinc Blende structure with F_{43m} space group symmetry, but in this calculation we have selected P_1 symmetry to make it a surface supercell structure. A systematic replacement of P atoms by Sb atoms leads to the formation of $\text{InP}_{1-x}\text{Sb}_x$ supercell structures. In the interstitial region of these structures, a plane wave cut-off parameter, $R_{\text{MT}}K_{\text{max}} = 7$ has been constantly maintained; where, R_{MT} is the average radius of the muffin-tin

(MT) spheres and K_{max} is the plane wave cut-off parameter. Inside the atomic spheres, a maximum value of angular momentum, $l_{\text{max}}=10$, has been maintained constant for expansion of the wave functions. The separation between the valence and the core energy states has been considered to be - 6.0 Ry. The calculation has been iterated until the total energies are converged below 10^{-5}Ry with respect to the Brillouin zone integration. The presence of Sb atoms in $\text{InP}_{1-x}\text{Sb}_x$ supercell, triggers the inclusion of relativistic effect of spin-orbit coupling (SOC) in these structures. The SOC effect has been performed along¹ direction for $\text{InP}_{1-x}\text{Sb}_x$ supercell structures. The necessary parameters obtained from such computation of $\text{InP}_{1-x}\text{Sb}_x$ supercell structures, are fed into BoltzTraP code¹⁹ which employs semi-classical Boltzmann Transport Equation (BTE) for calculation of transport parameters of the material, at constant relaxation time approximation.

3. Results and Discussions

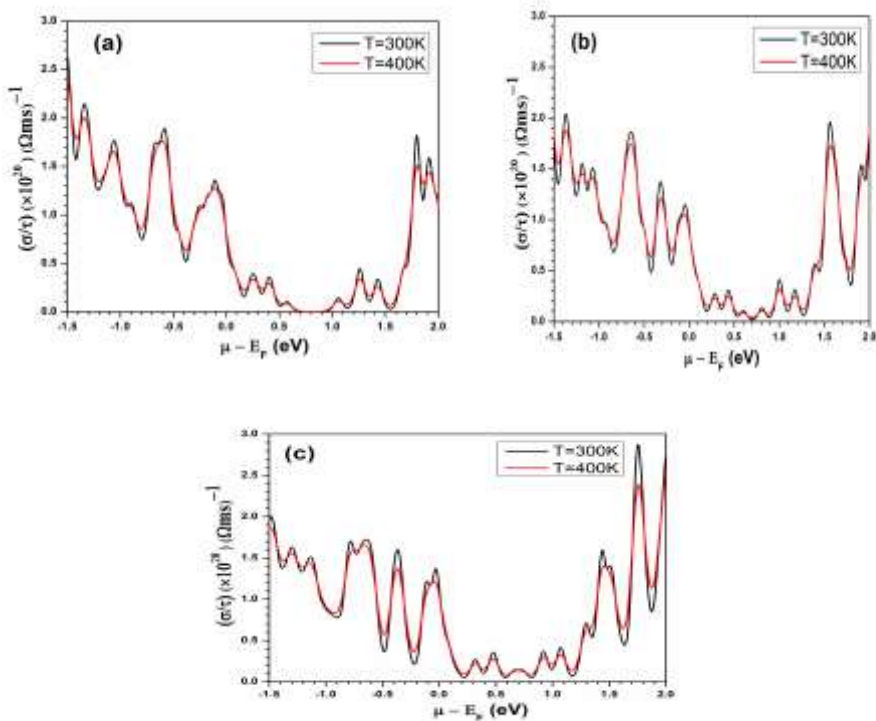


Figure 1. Variation of electrical conductivity at constant relaxation time approximation (σ/τ) as a function of chemical potential (μ) (with respect to Fermi Energy (E_F)), for $\text{InP}_{1-x}\text{Sb}_x$ supercell structures at (a) $x = 0.25$, (b) 0.50 and (c) 0.75 .

Figure 1 (a), (b) and (c) depicts the variation of electrical conductivity (σ) (at constant relaxation time approximation) as a function of chemical potential (μ) (with respect to Fermi Energy (E_F)) for $\text{InP}_{1-x}\text{Sb}_x$ supercell structures at $x = 0.25, 0.50$ and 0.75 , respectively. The electrical conductivity (σ) has been calculated with respect to relaxation time (τ), which is a linear phenomenon within the relaxation time approximation as implemented by BTE²³. The evaluation of τ becomes complex due to various scattering mechanisms (i.e., carrier scattering, phonon scattering, defect scattering, and boundary scattering). Moreover, τ satisfies the power approximation relationship and is both temperature and energy dependent²⁴, can be expressed as

$$(3.1) \quad \tau(E, T) = \tau_0 \left(\frac{E}{K_B T} \right)^{\frac{1}{2}},$$

where, E represents the energy band gap of the material and τ_0 is constant. The chemical potential (μ) has been calculated with respect to Fermi Energy (E_F)¹¹. The negative (positive) values of μ calculated with respect to E_F represent the valence (conduction) band sides. The chemical potential profile regards to the distribution of carrier density²⁵ along the bands (i.e., both conduction and valence). Thus, with increasing μ along both the bands (i.e., valence and conduction) σ is observed to encounter distinct peak values. With increasing Sb incorporation, the magnitude of σ peaks increases significantly along both the bands (specifically, along conduction band). Hence, such a diffusive transport mechanism can be explained as²⁶,

$$(3.2) \quad \sigma = \int \sigma(E) f'(E - E_F) dE,$$

where, f' is the energy derivative of Fermi function and $\sigma(E)$ represents the energy dependent transport function related to conductivity. The peak values of σ decreases with increase in temperature, at constant percentage of Sb incorporation in $\text{InP}_{1-x}\text{Sb}_x$ supercell structures.

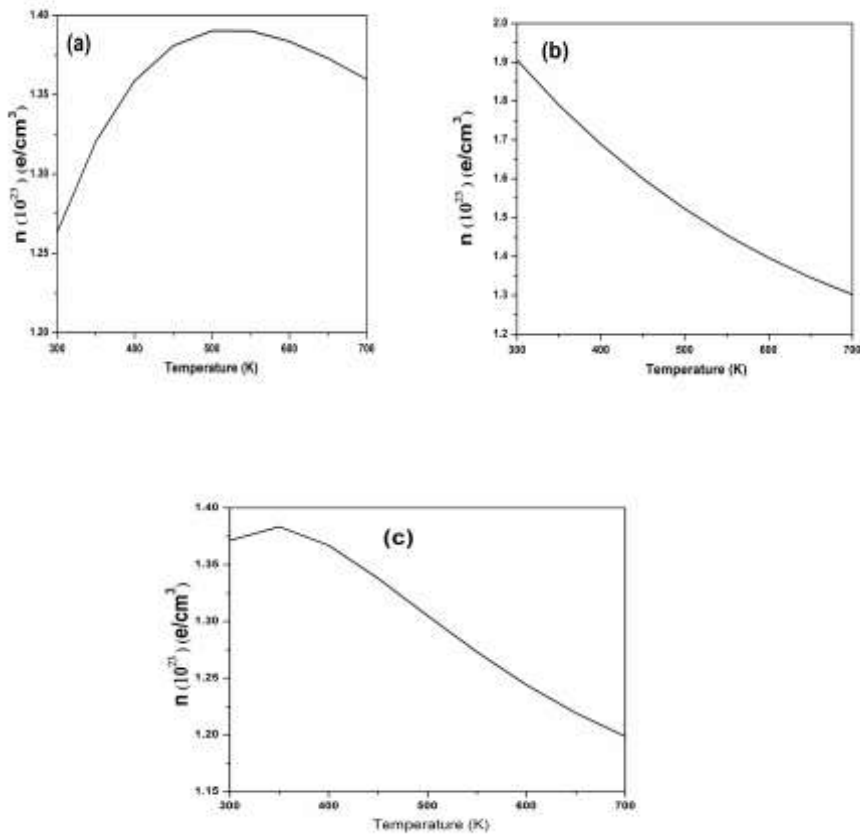


Figure 2. Variation of carrier concentration (n) as a function of temperature (T), for $\text{InP}_{1-x}\text{Sb}_x$ supercell structures at (a) $x = 0.25$, (b) 0.50 and (c) 0.75 .

Figure 2 (a), (b) and (c) illustrates the variation in carrier concentration (n) as a function of temperature (T) for $\text{InP}_{1-x}\text{Sb}_x$ supercell structures at $x = 0.25$, 0.50 and 0.75 , respectively. The carrier concentration is observed to increase with rise in temperature at lower percentage of Sb incorporation signifying an increase in kinetic energy of free charge carriers. A segment of carrier concentration characteristic curve where the value is observed to be almost constant signifies an enhancement of free carriers in conduction band. Whereas, the lowering nature of the carrier concentration curve at higher temperature for increased Sb incorporation illustrates the impact of impurity scattering due to the enhanced replacement of P atoms by higher atomic size Sb atoms in $\text{InP}_{1-x}\text{Sb}_x$. Although slope of carrier concentration curve falls at a significantly higher rate at elevated temperatures for intermediate Sb incorporation in comparison to its extremum.

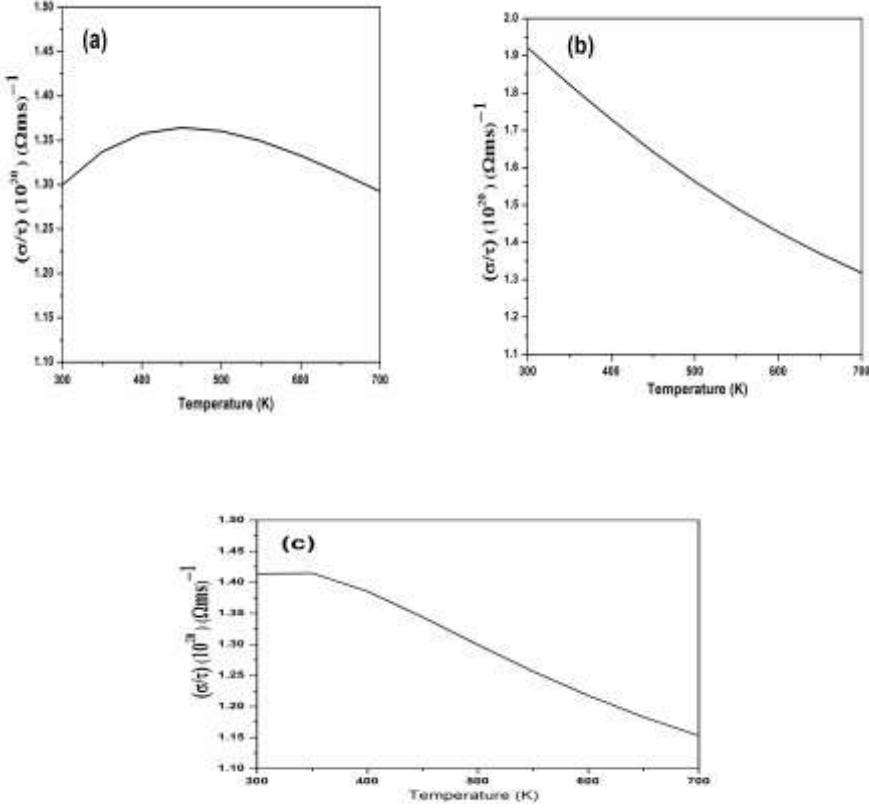


Figure 3. Variation of electrical conductivity at constant relaxation time approximation (σ/τ) as a function of temperature (T), for $\text{InP}_{1-x}\text{Sb}_x$ supercell structures at (a) $x = 0.25$, (b) 0.50 and (c) 0.75 .

The electrical conductivity (σ) defines the contribution of carriers in the flow of current in a material. The σ values calculated assuming constant relaxation time (τ) approximation as a function of T is depicted in figure 3 (a), (b) and (c) for $\text{InP}_{1-x}\text{Sb}_x$ supercell structures at $x = 0.25$, 0.50 and 0.75 , respectively. The σ is directly proportional to n^{27} as expressed by the following relationship

$$(3.3) \quad \sigma = ne\mu_e,$$

where, μ_e signifies the mobility of electrons.

Thus, the electrical conductivity characteristic curve is observed to imitate the nature of carrier concentration curve.

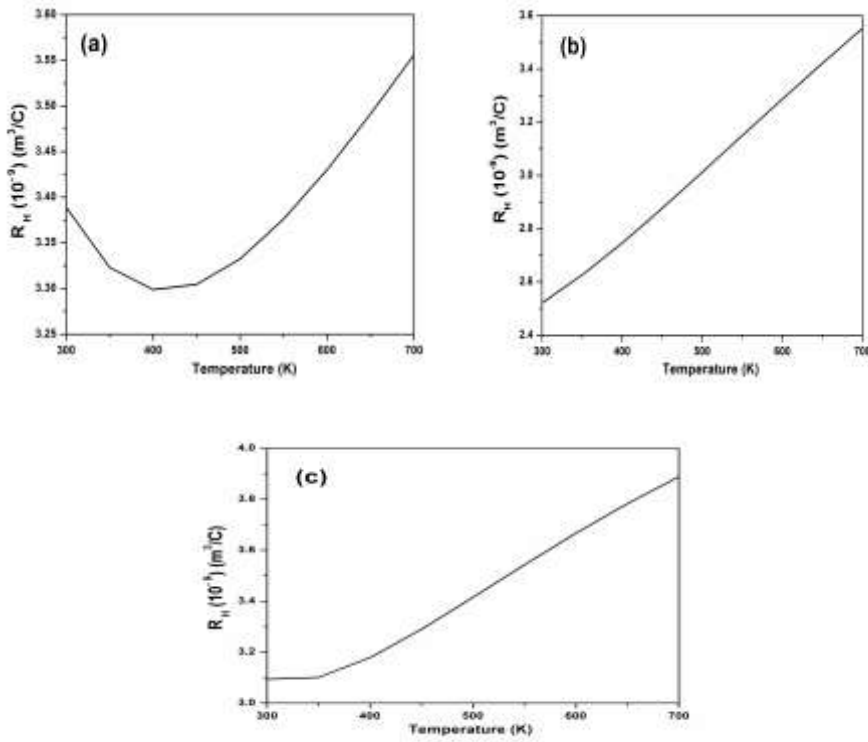


Figure 4. Variation of Hall coefficient (R_H) as a function of temperature (T), for $\text{InP}_{1-x}\text{Sb}_x$ supercell structures at (a) $x = 0.25$, (b) 0.50 and (c) 0.75 .

The variation of Hall coefficient (R_H) as a function of temperature (T) for $\text{InP}_{1-x}\text{Sb}_x$ supercell structures at $x = 0.25$, 0.50 and 0.75 are depicted in figure 4 (a), (b) and (c), respectively. The R_H values for all the characteristic curves are found to be negative which implies the contribution of electrons in the production of Hall voltage due to the application of magnetic field. Although in the characteristic curved the magnitude of R_H values have been considered. Moreover, the contribution to Hall coefficient by charge carriers (i.e., electrons and holes) observed to be nearly equal at intermediate Sb incorporation but varies negligibly at the extremum. R_H can be expressed by the following relationship²⁸

$$(3.4) \quad R_H = \frac{p\mu_h^2 - n\mu_e^2}{[e(p\mu_h + n\mu_e)]^2},$$

where, $n(p)$ and $\mu_n(\mu_p)$ represents electron (hole) and electron (hole) mobility, respectively. Thus, at lower percentage of Sb incorporation in

$\text{InP}_{1-x}\text{Sb}_x$, the R_H values are observed to decrease at lower temperatures in contrary to increasing carrier concentration. But, at higher Sb incorporation with elevated temperature, R_H values are observed to significantly increase due to the contribution from complicated multiband behavior²⁹.

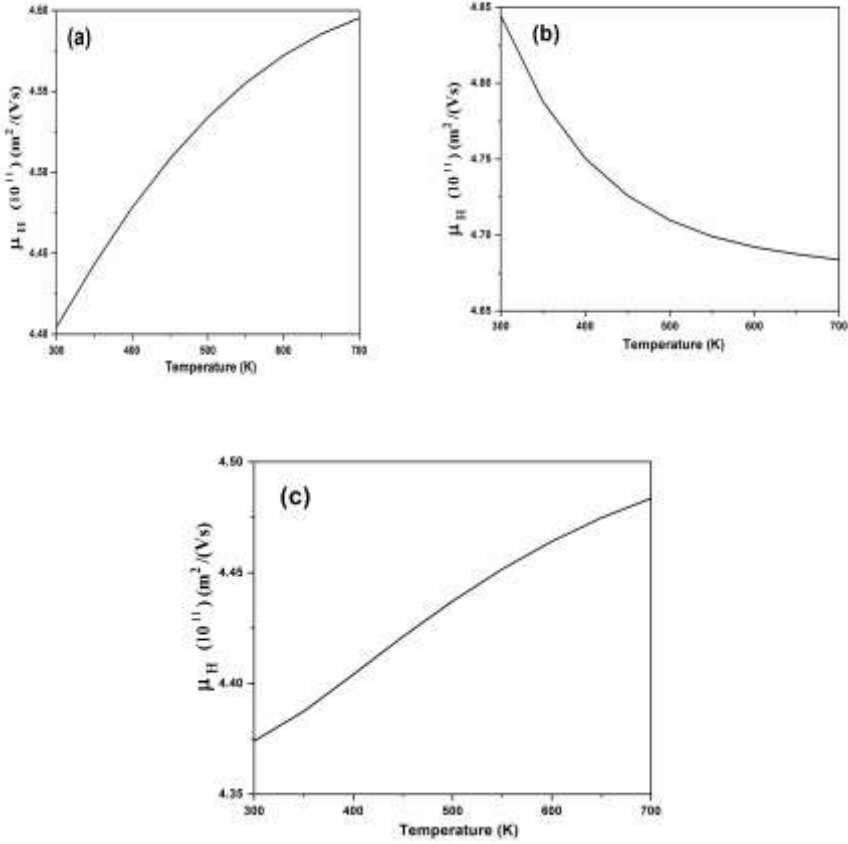


Figure 5. Variation of Hall mobility (μ_H) as a function of temperature (T), for $\text{InP}_{1-x}\text{Sb}_x$ supercell structures at (a) $x = 0.25$, (b) 0.50 and (c) 0.75.

The variation of Hall mobility (μ_H) as a function of temperature (T) for $\text{InP}_{1-x}\text{Sb}_x$ supercell structures at $x = 0.25$, 0.50 and 0.75 are depicted in figure 5 (a), (b) and (c), respectively. μ_H can be expressed as³⁰

$$(3.5) \quad \mu_H = \frac{R_H}{\rho},$$

where, ρ represents electrical resistivity of the material.

The increasing slope of μ_H observed for the extremum Sb concentration in comparison to that of intermediate concentration in $\text{InP}_{1-x}\text{Sb}_x$ supercell, signifies an enhanced phonon scattering in the structures.

4. Conclusion

The transport properties of $\text{InP}_{1-x}\text{Sb}_x$ supercell structures at $x = 0.25$, 0.50 and 0.75 has been computed employing BoltzTraP code. The chemical potential (μ) at various percentage of Sb incorporation in $\text{InP}_{1-x}\text{Sb}_x$ provides information regarding the carrier density distribution profile along the bands (i.e., both conduction and valence). At lower temperatures, the extremum values of Sb incorporation, has evolved rise in kinetic energy of the carriers; whereas, at elevated temperature the carrier concentration curve lowers signifying presence of impurity atoms with larger atomic size, in comparison to its counterpart. Mobility characteristic curve along the temperature range is observed to imitate the nature of carrier concentration curve. The Hall coefficient values are found to be negative (positive) indicating contribution from electrons (holes). The contribution of charged carriers (i.e., both electrons and holes) to Hall coefficient is obtained to be nearly equal and negligibly dissimilar at intermediate and extremum percentage of Sb incorporation in $\text{InP}_{1-x}\text{Sb}_x$, respectively. Interestingly, the Hall coefficient curve rises significantly at elevated temperatures. implying contributions from complicated multiband behavior. The occurrence of augmented slope in Hall mobility characteristic curve for entire temperature range at extremum Sb incorporation in $\text{InP}_{1-x}\text{Sb}_x$ structure, suggests phonon scattering effect in the material. This comprehensive computational study of the transport properties of $\text{InP}_{1-x}\text{Sb}_x$ at various percentage of Sb incorporation will urge to perform future experimental investigation on this material.

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