Correlation Between Bands Structure and Quantum Magneto Transport Properties in InAs/Ga$_x$In$_{1-x}$Sb Type II Superlattice for Infrared Detection

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We have used the envelope function formalism to investigate the bands structure of LWIR type II SL InAs (d$_1$ = 2.18 d$_2$)/In$_{0.25}$Ga$_{0.75}$Sb (d$_2$ = 21.5 Å). Thus, we extracted optical and transport parameters as the band gap, cut off wavelength, carriers effective mass, Fermi level and the density of state. Our results show that the higher optical cut-off wavelength can be achieved with smaller layer thicknesses. The semiconductor-semi metal transition was studied as a function of temperature. Our results permit us the interpretations of Hall and Shubnikov-de Haas effects. These results are in agreement with experimental results in literature and a guide for engineering infrared detectors.

Keywords: bands structure, quantum magneto transport, Shubnikov-de Haas effect, density of states, InAs/Ga$_x$In$_{1-x}$Sb superlattice, infrared detection

INTRODUCTION

There are a several efforts in developing infrared materials for Very Long Wavelength Infrared (VLWIR) photodetection with the optical cut-off wavelengths $\lambda_c \geq 7.5 \mu m$ in the atmospheric window. Currently, InAs/In$_{1-x}$Ga$_x$Sb type-II superlattices (SLs) are still the most promising candidate. In this area, Smith and Mailhiot [1] have shown that this material system provides distinctive advantages suitable for VLWIR photodetection.

The key lies in the fact that by increasing indium composition in In$_{1-x}$Ga$_x$Sb layer, the corresponding lattice constant increases. As a result, the tension in the InAs layer lowers the conduction subbands ($E_c$) whereas the compression in the In$_{1-x}$Ga$_x$Sb layer raises the heavy hole subband (HH$_i$). Therefore, a very smaller band gap can be optimized with a reasonably thinner period which is not possible in InAs/GaSb SL [2]. The most important advantage of this SL lies in the fact that the presence of strain within this SL layers reduces the Auger recombination process and improves significantly the carrier lifetime and detectivity [3]. We note that in the previous years, a very few works were reported to verify the theoretical performance of InAs/InGaSb SLs for LWIR and VLWIR photodetection.

The applications of this technology are in military, automobile, aircraft safety, medical diagnosis, and in remote sensing systems [4].

The theory of band structure is necessary for describing the effects of external excitations on transport parameters and properties of optoelectronics devices [5]. Owing to this lack of studies, we have investigated the bands structure of presented LWIR type II SL InAs (d$_1$ = 47 Å)/Ga$_{0.75}$In$_{0.25}$Sb (d$_2$ = 21.5 Å) with d$_1$/d$_2$ = 2.186 along the wave vector $k_z$ in the growth
direction and $k_p(k_x,k_y)$ in-plane of the superlattice. We extracted useful electro-optical parameters like the optical cut-off wavelength, the effective mass of electrons and holes and their evolution with temperature. We found the point of semiconductor (SC) to Semimetal (SM) transition. We calculated the density of states without and with applied magnetic field and deduced the dimensionality and the limit of the quantification of the energy of electron gas.

**THEORY AND BAND STRUCTURE**

The general expression of dispersion relation of type-II SLs, within the envelope function formalism and effective mass approximation, is given by [6–9]:

$$
\cos (k_z d) = \cos (k_1 d_1) \cos (k_2 d_2) - \frac{1}{2} \left[ \cos \left( \frac{\xi + \frac{1}{8}}{\xi} \right) + \frac{k_p^2}{4k_1 k_2} \left( r + \frac{1}{2} - 2 \right) \sin (k_1 d_1) \sin (k_2 d_2) \right], \quad (1)
$$

In each host material, we used the six bands Kane Hamiltonian ($6\times6$ matrix) describing the $k\cdot p$ interaction of $\Gamma_6$ doublet $[S, m^2_p = \pm 1/2]$ for electrons) and $\Gamma_8$ quadruplet $[P, m^2_p = \pm 1/2]$ for light holes and $[P, m^2_p = \pm 3/2]$ for heavy holes. The spin-orbit coupling is too large, compared to the hosts gaps $\varepsilon_i$, so the $\Gamma_7$ doublet is neglected. With the help of the Bloch condition, the continuity of the envelope functions and their derivatives at the interfaces we obtain a system with solution Equation (1). The inferior limit of the validity of this model is $d_1 < 10 \text{ Å}$ and $d_2 < 10 \text{ Å}$ as indicated by Bastard [6], Andlauer and Vog [7], Masur et al. [8]. Here $k_x$ and $k_p(k_x,k_y)$ are the wave vector in the growth direction and in-plane of the superlattice. The origin of the energy $E$ has been chosen at the top of InAs valence band as shown in the Figure 1. In each host material and for a given energy, the two–band Kane model [10] gives the wave vector $(k_x^2 + k_y^2)$. Therefore, the energy $E$ of the light particles (electron and light hole) is given by:

$$
\begin{align*}
\frac{1}{2} m_p^2 \hbar^2 \left( k_1^2 + k_p^2 \right) &= (E - \varepsilon_1) \text{ for InAs} \\
\frac{1}{2} m_p^2 \hbar^2 \left( k_2^2 + k_p^2 \right) &= (E - \varepsilon_2 - \Lambda) \text{ for InGaSb}, \quad (2)
\end{align*}
$$

The expression of $\xi$ and $r$ in the Equation (1) are:

$$
\xi = \frac{k_1}{k_2} r \text{ and } r = \frac{E - \Lambda - \varepsilon_2}{E - \varepsilon_1}
$$

From the same Equation (1), the superlattice heavy holes minibands can be calculated with the following relations:

$$
\begin{align*}
\frac{1}{2} m_p^2 \hbar^2 \left( k_1^2 + k_p^2 \right) &= E \text{ for InAs} \\
\frac{1}{2} m_p^2 \hbar^2 \left( k_2^2 + k_p^2 \right) &= (E - \Lambda) \text{ for InGaSb}, \\
\xi &= \frac{k_1}{k_2} r \text{ and } r = \frac{(m_p^2 h^2)}{(m_p^2 h^2)}, \\
\end{align*}
$$

The direct band gaps parameters $\varepsilon_i$ ($i = 1$ and 2) used here, as a function of temperature, are given by the empirical expressions reported in Matossi and Stern [11] and Roth et al. [12]. $P_i$ is the Kane matrix element.

The heavy holes effective masses of InAs and In$_{0.25}$Ga$_{0.75}$Sb are, respectively $(m_{hh}^0)_{1} = 0.41 m_0$ and $(m_{hh}^0)_{2} = 0.42 m_0$, as given in Levinshintein et al. [13]. Here $m_0$ is the free electron mass.

In this work, we have used the valence band offset $\Lambda$ of 510 meV between heavy holes sub-bands edges of InAs and In$_{0.25}$Ga$_{0.75}$Sb [14]. The origin of energy is taken on the top of VB in InAs (Figure 1).

The computation of band structures consists of solving the general dispersion relation with the reported parameters. In the Equation (1), state energy exists if the right-hand side lies in the range $-1$ to 1. In other words, $-1 \leq \cos(k_z d) \leq 1$ which implies $-\pi/d \leq k_z \leq \pi/d$ in the first Brillouin zone, with $d = d_1 + d_2$ is the superlattice period. In the study of energy $E$ as a function of wave vector in the direction of growth $k_z$ ($k_p = 0$), the solving procedure consists of going with small steps of energy through the studied range. Then finding, for a given $E$, the value of $k_z$ which is root of the dispersion relations. The same procedure is used for studying $E$ vs. the in-plane wave vector $k_p$ ($k_z = 0$ and $k_z = \pi/d$).

**RESULTS AND DISCUSSIONS**

**Bands Structures, Band Gap, Cut Off Wavelength, and Carriers Effective Mass**

In the Figure 2, we have plotted the energy of conduction ($E_c$), light-hole ($h_l$), and heavy-hole ($HH_l$) subbands at the center $\Gamma(k_x = 0)$ and the limit ($k_z = \pi/d$) of the first Brillouin zone (FBZ) as a function of $d_1 = 2.18 d_2$ at 1.2 K. These results show that when $d_1$ increases, the width of $E_i$ and $HH_l$ deceases. In
addition, we can notice that the fundamental band gap energy \( E_g(\Gamma) = E_1(\Gamma) - \text{HH}_1(\Gamma) \) decreases when \( d_1 \) increases. Therefore, a crossover between \( E_1 \) and \( \text{HH}_1 \) takes place at the semiconductor (SC) to Semimetal (SM) transition point \( T_c(d_{1c} = 115.43 \text{ Å}, E_{1c} = \text{HH}_1c = 485.25 \text{ meV}) \).

In Figure 3, at a given temperature the \( E_g \) decreases when the valence band offset \( \Lambda \), between the top of the heavy hole bands in the two host materials, increases. The transition SC-SM occurs when \( E_g \) goes to zero.

The evolution of the cut off wavelength \( |\lambda_c| \) as a function of \( d_2 \) is shown in Figure 4. These results were calculated by using the expression:

\[
\lambda_c(\mu\text{m}) = \frac{1240}{E_g(\text{meV})}
\]

The dependencies of \( |\lambda_c(\Gamma)| \) on \( d_2 \) and temperature (T) are shown in Figure 4. The figure divides itself into two regimes: (i) For \( d_2 \leq d_{2c} \): for each T, \( \lambda_c(\Gamma, d_2) \) increases significantly with increasing \( d_2 \). When \( d_2 \) exceeds the critical value of \( d_{2c} \), \( E_1 \) is confounded with \( \text{HH}_1 \) at the SC-SM transition point where \( \lambda_c(\Gamma, d_{2c}) \) diverges. The critical \( d_{2c} \) decreases from 53.5 Å at 1.2 K to 37 Å at 300 K. Thus, the SC-SM transition goes to lower \( d_1 \) when T increases. (ii) For \( d_2 > d_{2c} \): \( E_1 \) falls completely below \( \text{HH}_1 \) and the SL shows an inverted bands structure with a SM conductivity. In this regime a reverse behavior was observed. The inset figure shows the sensitivity of \( E_g \) on T. This result shows that when T increases \( E_g \) shifts to lower energies with 0.21 meV/K. This is due to the fact that the thermal energy and electron-phonon interaction increase with T which lead to a reduction of the potential seen by electrons, leading to a reduced \( E_g \). In the investigated temperature range, the corresponding 7.46 ≤ \( \lambda_c(\mu\text{m}) \) ≤ 11.94 situates this sample in the LWIR region. The SL bands structure shown in Figure 5 was computed at 1.2 K along \( k_z \) and \( k_p \) the growth and in-plan directions, respectively. Along \( k_z \), the widths of \( E_1 \) and \( E_2 \), \( |E_i(k_z = \pi/d) - E_i(k_z = 0)| \),
were found to be 129 and 193 meV, respectively. The presence of such dispersion indicates three dimensional like behavior of electrons which is in agreement with the reported results of Mitchel et al. [15].

The energy as a function of $k_z$ shows that: along $k_z$, the bands $E_i$ and $h_i$ of the light particles are non-parabolic and the heavy holes bands $HH_i$ are parabolic; but along $k_p$, $E_1$ and $HH_1$ are parabolic but $h_1$ is non-parabolic. The theoretical effective mass in general turns out to be a tensor with nine components defined as [16]:

$$
\frac{1}{m_{ij}} = \frac{\hbar^2}{\partial^2 E(k)} \partial k_i \partial k_j
$$

(5)

From Figure 5 we calculated carrier’s effective mass of light particles: electrons $E_1$, light holes $h_1$ and heavy holes $HH_1$, in the direction of growth ($k_z$) and in plane ($k_p$) of this sample. Figure 6 shows that along $k_p$, $m_{HH1}^*(k_p) = -0.41 m_0$ whereas $m_{E1}^*(k_p)$ increases from 0.092 $m_0$ to 0.151 $m_0$ and $m_{h1}^*(k_p)$ decreases from −0.026 to −0.339 $m_0$ at $k_p = \pi/d$. Along $k_z$, $m_{E1}^*(k_z)$ and $m_{h1}^*(k_z)$ diverge at inflection points $k_z = 0.0269 \text{ Å}^{-1}$ and $k_z = 0.103 \text{ Å}^{-1}$, respectively. At these points the effective mass changes its sign, in electron and light-hole bands. The dashed vertical line indicate the $m_{E1}^*(k_p)$ = 0.0887 $m_0$ at the Fermi wave vector $k_F$. Rogalski [17] gives a larger electron effective mass $m^*/m_0 \approx 0.02 \text{–} 0.03$ in InAs/GaInSb SLs, compared to $m^*/m_0 = 0.009$ in HgCdTe alloy with the same bandgap $E_g \approx 100$ meV. These values are indicated without $d_1$, $d_2$, temperature and direction of the effective mass tensor. Our results at the center $\Gamma$ of the first Brillouin zone are $m_{E1}^*(k_p) = 0.092 m_0$, $m_{E1}^*(k_z) = 0.026 m_0$, $m_{h1}^*(k_p) = m_{h1}^*(k_z) = -0.026 m_0$, and $m_{HH1}^*(k_p) = -0.41 m_0$.

**Interpretations of Hall Effect, the Density of States, and the Dimensionality of Carrier’s Charges**

We used the carrier density $n$ as a function of the inverse of temperature measured in Mitchel et al. [18] and Haugan et al. [19]. In order to determine the band gap with accuracy, we plotted $nT^{-3/2}$ as a function of 1.000/T. This lead to an experimental band gap of $E_g = (95 \pm 8)$ meV in the intrinsic domain, which is in agreement with our 104 meV calculated at 300 K. The observed difference of 8.87 meV is due to the reduction of the gap by strain [1] and the input parameters considered here as well as fluctuations during the growth of SL which could affect $E_g$. Note that Szmulowicz [20] and Szmulowicz et al. [21, 22] have studied the band structures of InAs($d_1 = 43.6$ Å)/In$_{0.23}$Ga$_{0.77}$Sb($d_2 = 17.3$ Å) with $d_1/d_2 = 2.52$ and the origin of energy taken at the bottom of the conduction band in InAs. The InAs conduction band–GaSb valence-band overlap was taken to be 140 meV. The band gap in this structure was tailored to be 120 meV. Whereas, Mitchel et al. [15] told a calculated $E_g = 66.4$ meV for this same sample. It's a contradiction and in addition the temperature of calculation of the gap was not given. From carrier density vs. inverse of temperature [18, 19], we deduced the activation energy $E_a = 0.196$ meV at low temperatures in agreement with the magnitude of thermal activation energy $k_B T$ at 2.3 K.

We plot the measured mobility $\mu$, in Mitchel et al. [18] and Haugan et al. [19] vs. temperature in logarithmic scales. This shows that when $T$ increases, $\mu$ decreases as $T^{-1.5}$ indicating the interaction of electrons with phonons in the intrinsic regime. This result confirms a tridimensional electron gas.

For the superlattice $i$th mini-band, with energy width $AE(i) = E(i)_{\text{max}} - E(i)_{\text{min}}$, the density of states (DOS) can be expressed as [23]:

$$
\rho_D^{(i)}(E) = \begin{cases} 
\frac{m^*}{\pi^2 \hbar^2} k_z(f) (E) & E_{\text{min}} \leq E \leq E_{\text{max}} \\
0 & \text{otherwise}
\end{cases}
$$

(6)

The generalization of Equation (6) required a sum over all mini-bands:

$$
\rho_D(E) = \sum_{i=1}^{n} \rho_D^{(i)}(E)
$$

(7)

From the dispersion curves $E(k)$ in Figure 5, we have calculated the SL density of states (DOS) of the two lowest conduction minibands $E_i$ and the first valence subband $HH_1$ at 1.2 K. As seen in Figure 7, the DOS is quantized in term of $m^*/\pi\hbar^2d_i$ with the presence of large dispersion in $E_i$. This shows a significant interaction between InAs wells justified by the ratio $d_1 = 2.18 d_2$ in this sample.

At given temperature the Fermi level energy was obtained by the formula:

$$
E_F = E_{E1} + \frac{\hbar^2 k_F^2}{2m_{E1}}
$$

with

$$
k_F^{2D} = (2\pi T)^{1/2} \quad \text{and} \quad k_F^{3D} = (3\pi^2 n)^{1/3}
$$

(8)
In the sample $	ext{InAs}(d_{1}=17.3\ \text{Å})/	ext{In}_{0.23}\text{Ga}_{0.77}\text{Sb}(d_{2}=2.52\ \text{Å})$ with $d_{1}/d_{2}=2.52$. The width of HH$_{1}$ was 0.01 meV along $k_{z}$. Whereas, at 1.2 K, our calculated bands structure indicated $E_{F}=166.3$ meV, $\Delta_{E_{1}}=123$ meV, $\Delta_{E_{2}}=193$ meV, and $\Delta E(k_{z}=\pi/d)=169.4$ meV. The widths of HH$_{1}$ are 0.05 meV and 20.8 meV along $k_{z}$ and $k_{p}$, respectively. The band HH$_{1}$ is flat along $k_{z}$ in Figures 1, 5 along $q=k_{p}$ in Szmulowicz [20] and Szmulowicz et al. [21, 22]. These values are in the same range as those given by Mitchel et al. [18], Haugan, et al. [19], Szmulowicz [20], and Szmulowicz et al. [21, 22] except for the band gap given there without temperature.

**Interpretation of the Shubnikov-de Haas Effect and the Density of States With Magnetic Field**

We have calculated the Fermi level in this SL by using the magnetoresistance results reported in Mitchel et al. [15].

It is well-known that the oscillations of longitudinal magnetoresistance at very low temperatures and under high...
magnetic fields, due to the Shubnikov-de Haas effect (SdH), are periodic with respect to $1/B$ [24].

The inverse of the minima $1/B_m$ as a function of the entire N, Landau level index, is given by the formula:

$$\frac{1}{B_m} = \Delta \left( \frac{1}{B} \right) \left( N + \frac{1}{2} \right),$$

(9)

The straight line slope of (9) gives the period, $\Delta(1/B) = 1.16 \, T^{-1}$. The relation between $\Delta(1/B)$ and the electron concentration $n_{3D}$ for a 3D system is given by:

$$n_{3D} = \left( \frac{2 e^{\Delta_{1/B}}}{} \right)^{1/2} \left( \sum_{N_{\text{SL}}}^{N_{\text{SL}}+1} \frac{1}{\Delta} \right),$$

(10)

So at $T = 1.2 \, K$ the SL electron density is $n_{3D} = 4.53 \cdot 10^{15} \, \text{cm}^{-3}$. The later permits us to estimate the Fermi energy by:

$$|E_F - E_1| = \left| \frac{he}{m^*_E} \right| \Delta (1/B),$$

(11)

Here, $m^*_E(k_F) = 0.09 \, m_0$ is the electron effective mass at the Fermi wave vector, extracted from Figure 6. As seen in Figures 5, 7, $E_F = 576.87 \, \text{meV}$ and the SL has an $n$ type conductivity at $1.2 \, K$.

In their work of InAs/InGaSb SL magnetotransport properties, Levinshtein et al. [13] have shown that such SL shows Shubnikov-de Haas (SdH) effect. In the Figure 9 we show the calculated Landau levels (LL) energies of $E_1$ in the investigated SL. These results are obtained by transposing the quantification rule [25] of the wave vector in the plane of the SL in $E(k_p)$ plotted in Figure 5:

$$k_p^2 = \left( \frac{2N^{(i)} + 1}{B} \right),$$

(12)

with $N^{(i)}$ the Landau index of the mini-band

$$E_F = \frac{eB}{2m^*_E} \left( \frac{3\pi^2 B}{R_{xy} e N_{\text{SL}} (d_1 + d_2)} \right)^{2/3}$$

(13)

with $N_{\text{SL}} = 73$ is the SL number of periods. The Hall resistance has been calculated with the formulat: $R_{xy} = h/\nu N_{\text{SL}}$ and $\nu$ is the filling factor [26].

In the Figure 9, when the magnetic field increases, the crossover between the calculated LL energy and the Fermi level gives the same minima (at $B = 5.71, 4.13, 3.40, 2.73$ and $2.34 \, T$), of the Shubnikov-de Haas effect (SDH) oscillations of the transverse magneto-resistance measured by Mitchel et al. [15].

The Figure 10 represents the computed 3D density of states (DOS) of the first conduction mini-band of the investigated SL by using the following expression [24]:

$$\rho_{3D}(E,B_z) = \frac{|e| B_z}{8\pi^2 h^2} \sum_{N_{\text{max}}}^{N_{\text{max}}} \sum_{N_{\text{SL}}}^{N_{\text{SL}}} \frac{1}{E - \left( N^{(i)} + \frac{1}{2} \right) \hbar \omega_c},$$

(14)

As can be seen in the figure the DOS is inversely proportional to the square root of total energy and the spacing between LL increases with the applied magnetic field.
A condition for the observation of the SDH effect is that the separation $h\omega_c/(\omega_c = eB/m^*_{\text{eff}})$ is the cyclotron pulsation between LL must be superior to activation thermal energy $k_BT$. So here the magnetic field must be $B > k_BT/m^*_{\text{eff}}$, $T/h\omega = 0.9T$ for $T = 1.2K$ and $m^*_{\text{eff}} = 0.09m_0$. When $B < 0.9T$, the LLs disappear and $E_1$ is a continuum. This condition of quantum limit agrees well with our calculated DOS ($E_1$, B) in Figure 10.

We also calculated the transport scattering time $\tau_p = \mu_{\text{H}}m^*_{\text{eff}}/e = 0.52\text{ ps}$ for Hall mobility $\mu_{\text{H}} = 1.2\times10^4\text{ cm}^2/\text{Vs}$ measured at 1.2K by Mitchel et al. [18] and Haugan et al. [19] and our $m^*_{\text{eff}} = 0.09m_0$. This value of $\tau_p$ can be compared to the quantum relaxation time $\tau_q = 0.5\text{ ps}$ and $\tau_p = 2.34\text{ ps}$ measured in AlGaN/GaN two-dimensional electron gas [27].

Fuchs et al. [28] reported for the SL1 InAs($d_1 = 34.8\text{Å}$)/GaAsGaInSb($d_2 = 29\text{Å}$) with $d_1/d_2 = 1.2$, $8\mu\text{m} < \lambda_c < 12\mu\text{m}$ corresponding to 103 meV $\leq E_g < 155\text{ meV}$ from electroluminescence for 10K $\leq T \leq 240\text{ K}$. In the studied sample SL2 InAs($d_1 = 47.3\text{Å}$/Ga$_{0.8}$In$_{0.2}$Sb($d_2 = 21.5\text{Å}$) with $d_1/d_2 = 2.19$, the insert of Figure 4 shows $\lambda_c(T)$ with $7.46 < \lambda_c(\mu\text{m}) \leq 10.5$ and $118\text{ meV} \leq E_g < 166\text{ meV}$ for the same investigated temperature range. In particular at low temperature, $E_g(77\text{K},\text{SL1}) = 150\text{ meV}$ from measured dynamical impedance increases to $E_g(77\text{K},\text{SL2}) = 157\text{ meV}$ in agreement with the fact that $E_g$ increases when $d_1/d_2$ increases at a given temperature as seen in Figure 11. In the SL1, an electron effective mass of 0.03 $m_0$ for transport perpendicular to the SL plane was used in the band-to-band tunneling model. This effective mass is in agreement with our $0.026 m_0$ in the SL1, an electron effective mass of $0.03 m_0$ for transport perpendicular to the SL plane was used in the band-to-band tunneling model. This condition of quantum limit agrees well with our calculated DOS ($E_1$, B) in Figure 10.

All datasets generated for this study are included in the article/supplementary material.

**AUTHOR CONTRIBUTIONS**

NB: corresponding author doing the most of the article. AN: the supervisor is correcting the article. DB: help in the band gap calculation. AB, MB, SM, E-SE-S, and FC: help in calculation of masses effective and magnetotraport. All authors have contributed to this work and approved it for publication.
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**Conflict of Interest:** The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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