Optical Absorption and Photoluminescence in the Spherical InP/InSb/InP Core/shell/shell Nano Structure

Harutyunyan VA¹, Kazaryan EM¹ and Hayrapetyan DB¹²

¹Russian-Armenian University, H. Emin 123, 0051, Yerevan, Armenia
²Peter The Great Saint, Petersburg Polytechnical University, Polytechnic heskaya 29, St. Petersburg, 195251, Russia

Abstract
The one particle states of charge carriers are considered in InP/InSb/InP core/shell/shell spherical quantum nano structure at the regime of strong quantization. The results of numerical calculations for the values of the energy of charge carriers for different values of the thickness of the quantizing layer of InSb are presented. The calculations were performed with allowance for the Kaned ispersion for electrons and light holes in the InSb layer. The dependence of the number and position of the energy levels of charge carriers in the quantizing layer of InSb on the width of the well (layer thickness) is shown. The dependence of the absorption coefficient and photoluminescence spectra on the energy of incident light of interband transitions have been investigated. The oscillator strengths and selection rules for these transitions have been obtained. The absorption has a strictly resonant character. By the orbital and azimuthal numbers only diagonal inter band transitions are possible. For the radial number, the transitions between the states with the same radial numbers have the highest intensity.

Keywords: Core/shell/shell, Spherical Quantum Layer, Size Quantization, Optical Absorption, Photoluminescence

Introduction
Indium antimonide (InSb) is the only semiconductor material, which can be used for three types of photo detectors: photo conductive (photo resistance), photo voltaic and photo electro-magnetic. It is one of the main materials for photo detectors, which operates in the range of 3-5 m. The unique properties of InSb make it possible to use it in the broadband of civil applications including medicine and ecological monitoring [1]. The optical properties of InSb have, of course, been long studied and are well understood [2]. There is no doubt that the presence of unique features, such as narrow band gap, high carrier mobility etc. [3], the size quantization fact or opens new opportunities for the device application of InSb. Hence, InSb remains significantly interesting material for the fundamental investigation of its nanostructure for potential application, such as kind nano electronic devices [3]. Nowadays quantum wells (films) [4], quantum wires [3,5] and quantum dots [6] on the basis of InSb have wide range of applications. At the same time, in the last two decades spherically symmetrical semi conductor hetero phase core/shell/shell structures [7-12] are also intensively studied. This is due to the fact that the increasing application of nano materials requires the development of new materials and structures. The requirements dictate that these materials and structures be capable of performing several tasks and functions within the frame work of the unified nanometric geometry [13-17]. In particularly, spherically symmetrical core/shell/shell structures simultaneously combine and synthesize in itself a number of properties of both quantum dots and quantum films. In the point of view of device application they are more multi-functional than the separate single quantum films and quantum dots [18,19]. In this regard, one of the technically realizable and promising for the application of core/shell/shell structures based on InSb is spherically symmetrical composition of InP/InSb/InP [20]. Let us note that in several works the electronic and optical effects are considered via various approximations in single spherical nano layer of InSb [21-23]. However, the consideration and quantitative description of electronic states and optical transitions have not performed yet in InSb nano layer, which is a component of real hetero phase InP/InSb/InP structure.

In the present work, the calculations of charge carrier’s energetic spectrum in the InSb nano layer of InP/InSb/InP spherical hetero composition are presented, as well as the results of theoretical investigation of optical absorption and photoluminescence in such layer are shown.

One-Particle States in InSb Nano layer of Spherical Hetero Composition InP/InSb/InP
Before presenting one-particle state calculations, let us present the basic physical characteristics of bulk crystals InP and InSb.
Table 1: The basic physical characteristics of bulk crystals InP and InSb [24-28]

<table>
<thead>
<tr>
<th>Material</th>
<th>Lattice constant ( a_0 (\text{nm}) )</th>
<th>Bandgap ( E_g ) (eV)</th>
<th>Exciton radius ( a_{\text{ex}} (\text{nm}) )</th>
<th>Electron affinity ( \Phi_{\text{e}} ) (eV)</th>
<th>Electron effective mass ( \mu_e / m_0 )</th>
<th>Heavyhole effective mass ( \mu_{lh} / m_0 )</th>
<th>Lighthole effective mass ( \mu_{lh} / m_0 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>InP</td>
<td>0.58687</td>
<td>1.344</td>
<td>10.15</td>
<td>-4.38</td>
<td>0.08</td>
<td>0.6</td>
<td>0.089</td>
</tr>
<tr>
<td>InSb</td>
<td>0.6479</td>
<td>0.17</td>
<td>65</td>
<td>-4.59</td>
<td>0.0145</td>
<td>0.43</td>
<td>0.015</td>
</tr>
</tbody>
</table>

Here \( m_0 \) is the mass of free electron. As it can be seen from the Table 1, the band off sets of energy on the interface of contacting materials are \( \Delta U = 0.21 \text{ eV} \) and \( \Delta U = 0.964 \text{ eV} \) for the conduction and valence bands, respectively. For instance, in this case the InSb nanolayer of the composition \( \text{InP/InSb/InP} \) is presented as a potential well with \( \Delta U = 0.21 \text{ eV} \) and \( \Delta U = 0.964 \text{ eV} \) for electron in the conductor band and for hole states in valence band, respectively.

In spherical coordinates \( (r, \theta, \phi) \), the total wave function of the particle \( \psi (r, \theta, \phi) \) will be found in the following form:

\[
\Psi (r, \theta, \phi) = \Phi (r) Y_{\ell m} (\theta, \phi) = \frac{Z(r)}{r} Y_{\ell m} (\theta, \phi)
\]

(3)

Here \( Y_{\ell m} (\theta, \phi) \) are the normalized spherical functions, and \( \ell = 0, 1, 2,... \) are the orbital and azimuthal quantum numbers, respectively [31].

Before proceeding to the specific calculations, let us adjust corresponding designations and the values of the parameters, which will be used in following numerical calculations.

For \( \text{InP} \): \( a_{\text{ex}} = a = 12 \text{ nm} \); \( \mu_e = \mu_{lh} = 0.08 m_0 \); \( \mu_m = \mu_{hh} = 0.1 m_0 \); \( \mu_{hh} = 0.6 m_0 \).

For \( \text{InSb} \): \( a_{\text{ex}} = a = 60 \text{ nm} \); \( \mu_e = \mu_{lh} = 0.0145 m_0 \); \( \mu_m = \mu_{hh} = 0.0145 m_0 \); \( \mu_{hh} = 0.5 m_0 \).

In this problem \( a = 12 \text{ nm} \) will be as a length unit, and \( E_{\text{max}} = \frac{\hbar^2}{2 \mu_{\text{ex}}} = 3.315 \times 10^{-3} \text{ eV} \) as an energy unit.

Let’s denote the inner and outer radii of the InSb layer by \( R_i \) and \( R_o \), respectively, and \( L=R_o - R_i \) is the thickness of the layer. In the calculations, the layer’s thickness varies in the range \( 0 \text{ nm} \) to \( 24 \text{ nm} \). It is clearly seen from the Table 1 that in the InSb layer the Coulomb interaction between the electron and hole can be neglected for such values of the layer’s thickness. That is, in the case under consideration the strong size quantization regime will be realized with sufficient accuracy for the charge carriers in the InSb layer. The value of the layer thickness \( L = 24 \text{ nm} \) is, in fact, the maximum permissible, when a strong quantization regime realizes in InSb layer. All calculations are made in the effective mass approximation.

Let us InSb layer approximate by rectangular potential well with finite depth in the radial direction. It can be written for the potential energy of the particle:

\[
V (r) = \begin{cases} 
\Delta U_{\text{ex}}, & 0 \leq r \leq R_i, r \geq R_o, \\
0, & R_i \leq r \leq R_o.
\end{cases}
\]

(1)

In this model, we now consider the single-particle states of charge carriers in InSb layer.

As it is known, in InSb Kane dispersion law occurs for electrons (also for light holes), which has the following for min the two-band model [29,30]:

\[
E_{\ell m} = \sqrt{\mu_{lh}^2 s^2 + \mu_{lh}^2 s^2 }; \quad s \sim 10^8 \text{ m/s}
\]

(2)

Here \( \mu \) is the full momentum of the particle. In the core and outer layer (InP) carrier dispersion law will be assumed strongly quadratic.

In spherical coordinates \( (r, \theta, \phi) \), the total wave function of the particle \( \psi (r, \theta, \phi) \) will be found in the following form:
In the case of electrons for the parameters \( a \) and \( b \) the following expressions were obtained:

\[
a = k_{e,2} = \sqrt{0.00364\varepsilon_{e}^2 - 2.255}, \quad b = k_{e,1} = \sqrt{63.35 - \varepsilon_{e}}.
\]

Derivative Bessel functions are calculated by the full argument.

The size quantization effect, as it is known, is mostly pronounced for the lower energy states of the charge carriers. Accordingly, we are interested in the several first solutions of the equation (10), which correspond to small values of quantum numbers. Consider the case of a relatively thin layer for visual clarity, when the number of states in the quantum well is not large.

In the Table 2 presented solutions of equation (10) illustrate the dependence of the electron energy levels and their position in the InSb quantum well when changing the layer thickness in the range of \( L \leq 15 \) nm. The calculations are made for the fixed value of the core radius \( R = 12 \) nm (\( \rho = 1 \)) and the depth of the well \( \Delta U_e = 0.21 \) ev.

### Table 2: Variation of the number of electronic energy levels in the InSb quantum well layer by changing the layer thickness in the range of \( L \leq 15 \) nm.

<table>
<thead>
<tr>
<th>Layer's thickness ( L ) (nm)</th>
<th>Number of levels</th>
<th>Energy ( E_{\text{el}} ) (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( L = 2.33 )</td>
<td>1</td>
<td>( n=1, l=0; \quad E_{1,0} = 105.38 )</td>
</tr>
<tr>
<td>( L = 3.29 )</td>
<td>2</td>
<td>( n=1, l=0; n=1, l=1; \quad E_{1,0} = 100.21, E_{1,1} = 105.68 )</td>
</tr>
<tr>
<td>( L = 4.57 )</td>
<td>3</td>
<td>( n=1, l=0; n=2, l=0; n=1, l=1; \quad E_{1,0} = 99.98, E_{2,0} = 197.77, E_{1,1} = 181.36 )</td>
</tr>
<tr>
<td>( L = 11.06 )</td>
<td>4</td>
<td>( n=1, l=0; n=2, l=0; n=1, l=1; n=1, l=2; \quad E_{1,0} = 91.20, E_{2,0} = 152.09, E_{1,1} = 138.93, E_{1,2} = 163.76 )</td>
</tr>
<tr>
<td>( L = 13.43 )</td>
<td>5</td>
<td>( n=1, l=0; n=2, l=0; n=1, l=1; n=2, l=1; n=1, l=2; \quad E_{1,0} = 89.11, E_{2,0} = 141.82, E_{1,1} = 130.98, E_{2,1} = 201.55, E_{1,2} = 150.17 )</td>
</tr>
<tr>
<td>( L = 15.36 )</td>
<td>6</td>
<td>( n=1, l=0; n=2, l=0; n=3, l=0; n=1, l=1; n=2, l=1; n=1, l=2; \quad E_{1,0} = 87.88, E_{2,0} = 135.08, E_{3,0} = 198.57, E_{1,1} = 125.47, E_{2,1} = 188.49, E_{1,2} = 146.06 )</td>
</tr>
</tbody>
</table>

As it is already noted, the dispersion law of light holes is also described by the expression (2) and, respectively, the energy levels of the light holes will also be determined from the expression of the form (10). The depth of the potential well for the hole states \( \Delta U_h = 0.964 \) ev is much greater than the depth of the well of the electronic states \( \Delta U_e = 0.21 \) ev). Accordingly, the number of quantum levels for hole states (in the case of both light and heavy holes) at the same layer thickness of the quantum well in the valence band is considerably more than the number of levels of electronic states. We will not give here for the hole state table similar to Table 2, and note only that the energy of hole states at the same layer thickness \( L \leq 15 \) nm when \( l=0 \) changes in the intervals of \( E_{\text{el}} \in [191.33 \text{ meV} \) and \( E_{\text{eh}} \in [0.01 \text{ meV} - 0.36 \text{ meV}] \) for the cases of light and heavy holes, respectively.

### Optical Absorption and Photoluminescence in InSb/InAs/InSb Nano Structure

Let us consider the inter band optical transitions in this core/shell/shell nano structure, when \( L = 24 \) nm. As noted above, it is the maximum range of thickness values when in InSb layer the exciton on effect can be neglected with sufficient accuracy.

Consider the dimension less oscillator strength, which is defined in the following way [33]:

\[
J = f_{e,\nu_e} / f_0 = \int \Psi_e(r_e) \Psi_h(r_h) dV
\]

Where \( f_0 \) is the oscillator strength of the bulk material, \( V_e = \{ n_e, l_e, m_e \} \) and \( V_h = \{ n_h, l_h, m_h \} \) are the sets of quantum numbers of the electron and light/or heavy hole, respectively. The values of the oscillator strength for the transitions from heavy and light hole states to the electron states are presented in the Table 3.

### Table 3: Values of the oscillator strength for \( |\nu_e\rangle \rightarrow |\nu_h\rangle \) inter band optical transitions, when \( R = 12 \) nm, \( \Gamma = 36 \) nm.

| \( n_{\text{eh}}=\{n_{\text{eh}},m_{\text{eh}}\} \rightarrow |n_{\text{eh}},l_{\text{eh}}\rangle \) | \( f_{\text{eh}} / f_0 \) | \( f_{\text{eh}} / f_0 \) |
|-------------------|------------|------------|
| Diagonal Transitions |
| \( |1,0\rangle \rightarrow |1,0\rangle \) | 0.9987 | 0.9998 |
| \( |2,0\rangle \rightarrow |2,0\rangle \) | 0.9736 | 0.9824 |
| \( |3,0\rangle \rightarrow |3,0\rangle \) | 0.9687 | 0.9601 |
| \( |1,1\rangle \rightarrow |1,1\rangle \) | 0.9955 | 0.9975 |
| \( |1,2\rangle \rightarrow |1,2\rangle \) | 0.9886 | 0.9973 |
| \( |2,1\rangle \rightarrow |2,1\rangle \) | 0.9754 | 0.9932 |
| \( |2,2\rangle \rightarrow |2,2\rangle \) | 0.9691 | 0.9816 |
| Non-diagonal Transitions |
| \( |2,0\rangle \rightarrow |1,0\rangle \) | 0.2417 | 0.1249 |
| \( |3,0\rangle \rightarrow |1,0\rangle \) | 0.1325 | 0.0291 |
| \( |1,1\rangle \rightarrow |2,1\rangle \) | 0.1284 | 0.1425 |
| \( |1,1\rangle \rightarrow |3,1\rangle \) | 0.0381 | 0.0525 |
| \( |2,1\rangle \rightarrow |1,1\rangle \) | 0.0067 | 0.0139 |
| \( |2,2\rangle \rightarrow |1,2\rangle \) | 0.0044 | 0.0048 |
| \( |3,1\rangle \rightarrow |1,1\rangle \) | 0.0018 | 0.0087 |

The presence in Exp.(3) of spherical functions \( Y_{lm}(\theta, \phi) \) leads by orbital and azimuthal quantum numbers to the selection rules \( l_e - l_h = 0 \) and \( |m_e - m_h| = 0 \), respectively.

Regarding the selection rules for the radial number \( n \), in Table 3 data demonstrate the following: transitions diagonally by radial number have the greatest intensity, and non-diagonal transitions are strongly suppressed (\( f_{\text{eh}} / f_0 \ll 1 \)). The intensity of the diagonal transition slowly decreases with increasing the values of both radial and orbital quantum numbers. The intensity of off-diagonal transitions decreases with increasing the degree of off-diagonality. So from a practical point of view, in the considered system inter band optical diagonal transitions by the radial number have a real interest. The threshold frequency of these transitions is determined by the relation...
Here $E_g$ is the band gap width of the bulk InSb sample, and $e, h$ a reset of quantum numbers of the electron and hole states, respectively. $\omega$ is frequency of the incident light. The main contribution in the band gap effective broadening

$$\hbar \omega_{e,h} = E_L^g + E_e + E_h$$  \quad (11)$$

$$\Delta_g = \hbar \omega_{e,h} - E_L^g$$  \quad (12)$$

Makes the radial quantized motion of the charge carriers. For a fixed value of the radial number, the variation of the band gap will be determined by the orbital number of charge carrier $l = l_c$. Table 4 shows the values of the effective broadening band gap of InSb layer for different inter band transitions.

**Table 4: Effective broadening band gap of InSb layer with different inter band transitions, when $R_1=12$ nm, $R_2=36$ nm.**

<table>
<thead>
<tr>
<th>Transitions</th>
<th>[(2,1)→(1,1)]</th>
<th>[(2,1)→(1,1)]</th>
<th>[(2,1)→(1,1)]</th>
<th>[(2,1)→(1,1)]</th>
<th>[(2,1)→(1,1)]</th>
<th>[(2,1)→(1,1)]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta_e^g$ (eV)</td>
<td>0.2497</td>
<td>0.3144</td>
<td>0.3793</td>
<td>0.3847</td>
<td>0.4071</td>
<td>0.5598</td>
</tr>
<tr>
<td>$\Delta_h^g$ (eV)</td>
<td>0.0962</td>
<td>0.1107</td>
<td>0.1265</td>
<td>0.1383</td>
<td>0.1541</td>
<td>0.1746</td>
</tr>
</tbody>
</table>

Now let us consider the inter band optical absorption in the real ensemble of core/shell/shell nanostructures with the dispersion of their sizes in the regime of strong size quantization. Note that this dispersion will lead to broadenings of spectral lines.

According to [34] we have following expression for light absorption coefficient for the strong quantization regime:

$$K(\omega) = K_0 \sum_{l_e, l_h} J^l \delta(\hbar \omega_{e,h} - E_L^g - E_e - E_h)$$  \quad (13)$$

Where $E_e$ is the energy gap of the semiconductor, $K_0$ is a quantity proportional to the square of modulus of the matrix element of the dipole moment taken over the Bloch functions. The broadenings of spectral lines will be taken into account with the help of replacing the delta function in expression (13) by Lorentz function:

$$\delta(\hbar \omega_{e,h} - E_L^g - E_e - E_h) \rightarrow \frac{\Gamma}{(\hbar \omega_{e,h} - E_L^g - E_e - E_h)^2 + \Gamma^2}$$  \quad (14)$$

Where $\Gamma$ - the width of Lorentzian parameter. For calculations we take $\Gamma=5\meV$ according to [35].

The next step of the investigation of the InP/InSb/InP Core/Shell/Shell structure's optical properties is the calculation of the photoluminescence (PL) spectra. The photoluminescence spectra is calculated using the Roosbroek-Shockley relation [36,37]:

$$R(\hbar \omega) = R_0 \hbar \omega K(\hbar \omega) \frac{f_e}{f_e - f_h}$$ \quad (15)$$

where $R_0$ is proportional to the square of modulus of the matrix element of the dipole moment taken over the Bloch functions, $f_e$ and $1 - f_h$ are probabilities of the conduction band states being occupied and the valance band states being empty, respectively. For the high temperatures the term $\frac{f_e}{f_e - f_h}$ in Roosbroek-Shockley relation transforms into the Boltzmann like form.

**Discussion of Results**

Let us now consider the results obtained with reference to optical inter band transitions in the structure under study. The results presented in Table 3 clearly show that the quantum size effect in this structure is especially pronounced in the InSb nano layer of the general structure of the core/shell/shell. Indeed, for transitions between states with identical radial numbers (Fig.1, Fig.3), the absorption has an essentially resonant character. Ideally (in the model of an infinitely deep well for the InSb layer), these peaks become delta-shaped needles of equal height. The intensity of transitions between states with unequal radial numbers is less, the greater the degree of non-diagonality of the transitions (Fig.2, Fig.4). In the same ideal, these curves simply disappear. Those, the results of the calculations show that the proposed model physically adequately describes the system under consideration and that in this hetero structure charge carrier localization due to size quantization occurs precisely in the InSb nano layer.
The dependence of the absorption curve for the diagonal transitions between heavy-hole and electron on the frequency of the incident light: 1) $|1,0\rangle \rightarrow |1,0\rangle$, 2) $|1,1\rangle \rightarrow |1,1\rangle$, 3) $|1,2\rangle \rightarrow |1,2\rangle$, 4) $|2,0\rangle \rightarrow |2,0\rangle$, 5) $|2,1\rangle \rightarrow |2,1\rangle$.

The dependence of the absorption curve for the off-diagonal transitions between heavy-hole and electron on the frequency of the incident light: 1) $|2,0\rangle \rightarrow |1,0\rangle$, 2) $|2,1\rangle \rightarrow |1,1\rangle$, 3) $|1,0\rangle \rightarrow |2,0\rangle$, 4) $|1,1\rangle \rightarrow |2,1\rangle$, 5) $|2,2\rangle \rightarrow |2,1\rangle$.

The Fig.1 and Fig.2 show the dependence of the absorption coefficient for the diagonal and off-diagonal inter band optical transitions, correspondingly, between light-hole and electron on the frequency of the incident light. The sets of the peaks correspond to the different quantum transitions. As the oscillator strengths for the diagonal transitions with a high accuracy are equal to one therefore the intensity values are the same for the all diagonal transitions. The opposite situation is observed for the off-diagonal transitions.

The Fig.3 and Fig.4 show the dependence of the absorption coefficient for the diagonal and off-diagonal inter band optical transitions, correspondingly, between heavy-hole and electron on the frequency of the incident light.

Note that the PL curves have been calculated for the room temperature. The separate peaks corresponding to the transitions described in the absorption part can be seen in the PL spectra. As we mention above for the high temperatures the term $\frac{g_{v}}{g_{c}}$ in Roosbroeck-Shockley relation transforms into the Boltzmann like form and this term vanishes the peaks in the high-energy region. That is why the low energy peaks can be observed more clearly in the PL spectra than the high-energy peaks [38,39]. It is also obvious that the peaks corresponding to the diagonal transitions have higher intensity than the peaks corresponding to the non-diagonal transitions.

The dependences of the PL intensity on the frequency of the incident light for the heavy-hole electron diagonal and non-diagonal transitions are shown in Fig. 5 and Fig. 6, respectively. As we can see from the PL spectra for light hole - electron and heavy-hole - electron transitions the intensity of the PL spectra increases with the increase of temperature. The same dependences of the PL spectra for the light-hole electron diagonal and non-diagonal transitions are shown in Fig. 7 and Fig. 8, respectively. Note that the intensity PL spectra increases with the increase of the temperature, while in experiments the opposite behaviour is observed. This is due to the fact that we have not considered the interaction of the exciton with phonons, the amount of which increases with the increase of temperature. In this case, the non-radiative recombination processes increases and the intensity of the PL spectra decreases.

Figure 5: The dependence of the photoluminescence intensity for light hole - electron diagonal transitions on the frequency of the incident light in arbitrary units.

Figure 6: The dependence of the photoluminescence intensity for light hole - electron non-diagonal transitions on the frequency of the incident light in arbitrary units.

Figure 7: The dependence of the photoluminescence intensity for heavy hole - electron diagonal transitions on the frequency of the incident light in arbitrary units.
Figure 8: The dependence of the photoluminescence intensity for heavy hole - electron off-diagonal transitions on the frequency of the incident light in arbitrary units.

**Conclusion**

Concerning the results obtained in the work, we can conclude the following:

- The model proposed in the paper physically adequately describes the states of charge carriers in the spherical hetero phase core/shell/shell structure of InP/InSb/InP in the strong-quantization regime.
- In the wide range of changes in the thickness of the InSb layer, in the layer the carrier states are described with sufficient accuracy by single-particle wave functions without taking into account the Coulomb interaction between the electron and the hole.
- In the same range, the thickness of the layer can be controlled in the controlled manner by the width of the band gap of the InSb layer, ie, it is possible to control the frequency of absorption- transmission of the incident light wave in a controlled manner.
- Along with the thickness of the layer, an important factor is also the large difference between the values of the effective masses of electrons and heavy holes in the frequency spectrum of inter band absorption. In this structure, this factor is one of the most important again due to the localization of charge carriers in the InSb layer.

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**References**

22. Amirkhanyan SM, Kazaryan EM, Sarkisyan HA (2015) Calculation of electro static multi poles of electron localized...
http://www.ioffe.ru/SVA/NSM/Semicond/InSb/basic.html
http://www.ioffe.ru/SVA/NSM/Semicond/InSb/bandstr.html