TYPE-II InGaAsP/GaAsSb NANO-SCALE HETEROSTRUCTURE

This chapter deals with the detailed study of type-II InGaAsP/GaAsSb nano-heterostructure and its optical responses by using k.p method. The reason behind the study of such heterostructures is to draw the great attention towards potential applications in the area of optoelectronic such as detectors, lasing heterostructures and optical sensors operating in the short wave infra red (SWIR), mid wave infra red (MWIR), and far infra red (FIR) regimes [1]. These heterostructures are also being utilized in molecular spectroscopy, pollution detection and its measurement, and trace-gas analysis. Moreover, the type-II heterostructures at nano-scale have exhibited high optical gain as compared to other type-I nano-scale heterostructures. Apart from the investigation of the optical response of such heterostructures, the effects of external parameters such as uniaxial external pressure or strain on optical gain spectra are also investigated. Prior to investigate the optical response such as optical gain of the heterostructure, $\bar{k},\bar{p}$ theory is adopted to find the envelope functions associated with carriers in the respective conduction and as well as valence band, probability densities or carrier densities, E-K curves of the quantum well of the heterostructure. The effect of variable temperature and application of external electric field on the heterostructure are also studied in order to determine the variations in gain characteristics under these parameters.

7.1 Structural Information of Type-II InGaAsP/GaAsSb nano-heterostructure

Under this section, the structural information of the Type-II InGaAsP/GaAsSb nano-scale heterostructure is given. The structure under study is a ‘W’-shaped type-II (staggered type) symmetric heterostructure and composed of InGaAsP and GaAsSb thin layers. The material GaAsSb (of thickness ~2 nm) is sandwiched between the materials InGaAsP (of thickness ~2 nm) and thus the heterostructure looks like InGaAsP/GaAsSb/InGaAsP layers which are again sandwiched been InP material, as shown in figure 1. In figure 1, it can be seen that the proposed heterostructure consists of two quantum wells of InGaAsP material but the conduction band offset value of these quantum wells is smaller than that of barrier (or space region). Similarly, the valence band offset value of these quantum wells is smaller than that of barrier (or spacer
The band offset values of the quantum wells and barrier has also been listed in table 1. This is the unique feature of this heterostructure which differentiate it from other heterostructures reported till date. This arrangement of the wells and the barrier in the heterostructure removes the restriction of choice of small bandgap materials (for QW formation) for the formation of heterostructures for emitting long wavelength radiations.

![Energy band profile of type-II InGaAs/GaAsSb nano-heterostructure.](image)

**Figure 1.** Energy band profile of type-II InGaAs/GaAsSb nano-heterostructure.

<table>
<thead>
<tr>
<th>S. No.</th>
<th>Layer Specification</th>
<th>Role of Layer</th>
<th>Conduction band-offset (eV)</th>
<th>Valence band-offset (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>$\text{In}<em>{0.5}\text{Ga}</em>{0.5}\text{As}<em>{0.8}\text{P}</em>{0.2}$</td>
<td>Quantum wells</td>
<td>0.190</td>
<td>0.263</td>
</tr>
<tr>
<td>2.</td>
<td>$\text{GaAs}<em>{0.5}\text{Sb}</em>{0.5}$</td>
<td>Barrier (Spacer)</td>
<td>0.330</td>
<td>0.483</td>
</tr>
<tr>
<td>3.</td>
<td>$\text{InP}$</td>
<td>Substrate</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

### 7.2 Computation of Envelope Functions and Probability density by k.p Method

Before the investigation of the optical properties of the designed type-II InGaAsP/GaAsSb nano-heterostructure, the knowledge of wavefunctions associated with carriers in the respective
conduction and as well as valence band, and localization of carriers (i.e. probability density of electrons and holes in conduction and valence band, respectively) is essential. So, keeping in views these all studies, the Schrödinger wave equation (taking into account the energy dependent electron effective mass) and $6 \times 6$ Kohn-Luttinger Hamiltonian have been solved for conduction and valence band solutions, i.e. for determination of the wavefunctions associated with the conduction subbands and valence subbands, respectively, of the heterostructure. By knowing the calculated wavefunctions, the actual localization (density) of the electrons and holes (light and heavy holes) can be determined because the carrier density is square of the ground state electron or hole wave function. While performing calculations, the calculations keep total angular momentum ($J$) as $3/2$, projection ($m_j$)=±1/2 and $m_j=±3/2$, respectively, for light holes and heavy holes and then expand the hole wave function in Luttinger-Kohn representation’s basis function. The required parameters in the calculations are listed in table 2. On completion of the entire calculations, the carrier’s density (localized electrons and holes) is obtained and thus the overall optimized energy band structure of ‘W’-shaped type-II InGaAsP/GaAsSb nanoscale heterostructure along with the localized electrons and holes associated with different regions of the heterostructure is shown in figure 2. In figure 2, the light black curve lines represent wavefunctions associated with e1, e2, hh1 and hh2 etc; while bold black curve lines represent total density of electrons and holes.

![Figure 2. Energy band diagram of InGaAsP/GaAsSb heterostructure showing localization of electrons and holes.](image-url)
Table 2. Parameters of materials used in designing InGaAsP/GaAsSb heterostructure [2, 3].

<table>
<thead>
<tr>
<th>Parameters</th>
<th>$\gamma_1$</th>
<th>$\gamma_2$</th>
<th>$\gamma_3$</th>
<th>Effective mass of electrons</th>
<th>Effective mass of holes</th>
</tr>
</thead>
<tbody>
<tr>
<td>InAs</td>
<td>20.0</td>
<td>8.50</td>
<td>9.20</td>
<td>$m_e = 0.026m_o$</td>
<td>$m_{hh} = 0.333m_o$</td>
</tr>
<tr>
<td>GaAs</td>
<td>6.98</td>
<td>2.06</td>
<td>2.93</td>
<td>$m_e = 0.067m_o$</td>
<td>$m_{hh} = 0.207m_o$</td>
</tr>
<tr>
<td>GaSb</td>
<td>13.4</td>
<td>4.70</td>
<td>6.00</td>
<td>$m_e = 0.039m_o$</td>
<td>$m_{hh} = 0.250m_o$</td>
</tr>
<tr>
<td>InP</td>
<td>5.05</td>
<td>1.6</td>
<td>2.1</td>
<td>$m_e = 0.0795m_o$</td>
<td>$m_{hh} = 0.60m_o$</td>
</tr>
<tr>
<td>GaP</td>
<td>4.05</td>
<td>0.49</td>
<td>2.93</td>
<td>$m_e = 0.09m_o$</td>
<td>$m_{hh} = 0.79m_o$</td>
</tr>
</tbody>
</table>

7.3 Optical Gain Characteristics of Type-II InGaAsP/GaAsSb Nano-Heterostructure

For the type-II InGaAsP/GaAsSb heterostructure, the optical gain has been studied for 2D carrier injection density of $5 \times 10^{12}$ /cm$^2$ and plotted against energy and wavelength, as shown in figure 3 (a) and (b). Figure 3 (a) shows the TE optical gain vs energy while figure 3 (b) shows the TE optical gain vs wavelength. In figure 3, it can be seen that the e1-h1 transition is the prominent transition and make significant contribution in the optical gain. The optical gain of the heterostructure under TE mode for e1-h1 transitions is found ~ 4013 /cm at energy 0.668 eV, as shown in figure 3 (a). Refer to figure 3(b), the peak optical gain is obtained at a wavelength of 1.853 µm. Optical gain is found to be significant in the wavelength range 1.75 to 1.9 µm.

![Figure 3](image-url)

Figure 3. Plot of optical gain (a) Energy dependent (b) wavelength dependent for 2D carrier injection density of $5 \times 10^{12}$ /cm$^2$. 

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7.4 Optical Gain Characteristics with variable mole fraction

Optical gain of the QW-heterostructure is further studied in TE polarization mode theoretically under 2D carrier density and with the antimonide (Sb) and arsenic (As) fraction variations. Figure 4 (a) shows the optical gain in TE mode vs Energy as Sb fraction variation from 0.3 to 0.7 with a constant As fraction = 0.8. Figure 4 (b) shows the optical gain in TE mode vs Energy as As fraction variation from 0.5 to 0.9 with a constant Sb fraction = 0.5. The peak value of optical gain is 3955 /cm at 0.669 eV for Sb fraction of 0.5 and As fraction of 0.8. Optical gain is found to rise with Sb and As fraction till an optimum value and continues to fall after that.

![Figure 4. TE Optical gain (a) with Sb fraction variation (b) with As fraction variation for 2D carrier injection density of 5x10^{12} /cm^2.]

7.5 Effect of Temperature on Optical Gain Characteristics

Figure 5 shows the optical gain in TE mode as temperature variation. Optical gain is calculated for temperatures ranging from 240K to 340K with an interval of 20K. A left shift along with a gradual fall is observed in the optical gain spectrum at carrier injection of 5x10^{12} /cm^2. The optical gain is also simulated for other range of temperature i.e. for the range of 0K to 300K for different carrier injection densities. Figure 6 shows the optical gain of type-II InGaAsP/GaAsSb nano scale heterostructure versus photonic energy for variable temperature ranging from 0K to 300K. Figure 5 and 6 show the similar variation in optical gain with variation in temperature. The effect
of temperature on optical gain and optical wavelength of the heterostructure has been summarized in figure 7. Figure 7 shows that optical gain decreases but the optical wavelength increases with increasing temperature.

**Figure 5.** TE Optical gain with variable temperature

**Figure 6.** Behavior of total optical gain of InGaAsP/GaAsSb heterostructure under variable temperature.
Figure 7. Effect of temperature on peak gain and optical wavelength.

7.6 Effect of Carrier Injection Density on Optical Gain Characteristics

Figure 8. TE Optical gain with variable carrier injection density
The Effect of injected carrier Density on optical gain spectra is shown in figure 8. Optical gain is calculated for 2D carrier densities of 5, 6, 7, 8 and \(9 \times 10^{12} \text{cm}^{-2}\) respectively. The optical gain of the heterostructure under TE polarization is \(4719 \text{ /cm under injected carrier density of } 6 \times 10^{12} \text{cm}^{-2}\) and \(6414 \text{ /cm under injected carrier density of } 9 \times 10^{12} \text{cm}^{-2}\). A right shift is seen in the optical gain spectrum under different carrier densities. A gradual rise in the optical gain spectrum is also seen with increasing carrier injection.

### 7.7 Effects of Uniaxial Pressure on Optical Gain Spectra

In order to see the uniaxial pressure effect of the optical gain spectra, external uniaxial strain is applied along [110] direction on the QW-heterostructure and the optical gain is calculated for external strains of 1, 5 and 10 GPa respectively. A left shift is observed in the optical gain spectrum under increasing strain. In figure 9, it is observed that the optical gain increases and as well as the operating energy shifts towards left side (towards longer wavelength) on applying the uniaxial strains of 1, 5 and 10 GPa along [110] direction. The optical gain of \(4700 \text{ /cm at } 0.65 \text{ eV under external strain of 10 Gpa and 3955 /cm at } 0.669 \text{ eV under no external strain condition is obtained. Thus a significant rise of } 745/\text{cm in optical gain spectrum is seen under uniaxial strain along [110] direction under TE polarization mode along with a corresponding left shift of 0.019 eV in energy.}

![Figure 9](image-url)
7.8 Effects of External Electric Field on Optical Gain Spectra

In order to understand the effect of external electric field on the optical gain and optical wavelength (photonic energy) of the heterostructure; the electric field is applied with the magnitude ranging from 20 to 200 KeV/cm. Figure 10 represents the relationship of optical gain of type-II InGaAsP/GaAsSb nano scale heterostructure versus photonic energy under the influence of different values of DC electric fields. Figure 10 shows that the peak of total optical gain and photonic energy of the emitted radiations is reduced significantly as the magnitude of the applied electric field is increased. Similar results have also been observed and explored under the applied electric field for type-I AlGaAs/GaAsP nanoscale heterostructure and InGaAs/GaAs strained quantum well heterostructure [4, 5]. In addition, broadening of the peak of the gain spectra is also observed with increasing the magnitude of the electric field. The effect of electric field on the optical gain spectra and optical wavelength of the type-II InGaAsP/GaAsSb heterostructure has also been summarized in figure 11. From figure 11, it can be seen that for the applied electric field ranging from 20 KeV to 200 KeV/cm, the peak gain has been reduced from 6551 cm\(^{-1}\) to 576 cm\(^{-1}\); while the wavelength has been shifted from 1.85 µm to 2.15 µm.

![Figure 10](image_url)

**Figure 10.** Behavior of total optical gain of InGaAsP/GaAsSb heterostructure under variable external electric field.
Figure 11. Effect of electric field on peak gain and optical wavelength.

References


5. W. J. Fan, “Band structures and optical gain of InGaAsN/GaAsN strained quantum wells under electric field”, Published in Electrical & Computer Engineering (ICECE), 2012, 7th International Conference on, IEEE xplore digital library, DOI: 10.1109/ICECE.2012.6471559, (2013).