CHAPTER 7

OPTICAL RESPONSE OF TYPE-I AlGaAs/GaAsP NANO-SCALE HETEROSTRUCTURE

This chapter deals with the detailed study of type-I GaAlAs/GaAsP nano-heterostructure and its optical responses by using k.p method. The effects of external parameters such as external electric field, variable temperature and uniaxial external pressure or strain on optical gain spectra are also investigated. Prior to investigate the optical gain of the heterostructure, k.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.

7.1 Structural Information of Type-I AlGaAs/GaAsP Heterostructure

In this section, the detail of the type-I AlGaAs/GaAsP nano-scale heterostructure is given. The proposed heterostructure under study consists of single quantum well of GaAs\textsubscript{0.84}P\textsubscript{0.16} with a barrier of Al\textsubscript{0.45}Ga\textsubscript{0.55}As. The heterostructure is supposed to be grown on GaAs substrate, as detailed in table 1. The choice of GaAs substrate is due to lattice matching with the quantum well layer and barriers.

<table>
<thead>
<tr>
<th>Layers Specification</th>
<th>Role of Layers</th>
<th>Energy Band gap (eV)</th>
<th>Lattice constants (Å)</th>
<th>Electron effective mass in conduction band</th>
<th>Strain</th>
<th>Conduction band edge-offset (eV)</th>
<th>Valence band edge-offset (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaAs\textsubscript{0.84}P\textsubscript{0.16}</td>
<td>Quantum well</td>
<td>1.616</td>
<td>5.6209</td>
<td>0.07429</td>
<td>0.005</td>
<td>0.284934 (at 100 K)</td>
<td>0.18668 (at 100 K)</td>
</tr>
<tr>
<td>Al\textsubscript{0.45}Ga\textsubscript{0.55}As</td>
<td>Barriers</td>
<td>1.983</td>
<td>5.6572</td>
<td>0.1394</td>
<td>-0.001</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>GaAs</td>
<td>Substrate</td>
<td>1.519</td>
<td>5.653</td>
<td>0.067</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
7.2 Computation of Envelope Functions and Probability density by k.p Method

Prior to investigate the optical gain of the designed AlGaAs/GaAsP heterostructure, the knowledge of wavefunctions associated with carriers in the respective conduction and as well as valence band, and their probability densities or carrier densities are very essential. In order to evaluate the behavior of the conduction band electrons wave functions and their corresponding discrete energies, the Schrodinger wave equation is solved taking into accounts semi-parabolic nature of conduction band and as well as effective-mass approximation. To evaluate the behavior valence band holes, the computations of their wavefunctions are required. These computations are much are complex rather than conduction band calculations. For such complex calculations, the k.p model has been used, as given in reference [1], which considers the $4 \times 4$ Luttinger-Kohn Hamiltonian. For the calculations of discrete energies of light and heavy holes (valence sub-bands), the $4 \times 4$ Hamiltonian with appropriate chosen basis is sufficient. All these calculations were performed in the vicinity of the zone centre at the $\Gamma$ point within the framework of the “Heterostructure Design Studio” software. Further the split-off holes were not considered because of its position lying at ~ 300 meV below the top of the valence band. Moreover, only two upper light holes and two upper heavy holes around $\Gamma$ point were calculated. These calculations generate the sufficient data for the description of complex valence band structure.

After the calculations of the wavefunctions associated with conduction band electrons and valence band holes, the carrier densities or probability densities of the electrons and holes lying in the active region of the $\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}/\text{GaAs}_{0.84}\text{P}_{0.16}$ nano-scale-heterostructure were calculated and plotted in figure 1. By calculating the wavefunction associated with any particle, the probability density of the particle can be calculated. Mathematically, the probability density of the charge carriers is defined as $P = |\psi^\dagger \psi|^2$. In figure 1, it is shown that the total probability density of electrons (shown by red color), which shows the localization of the electrons, in conduction band of active region or quantum well is highest at the central region; while the total probability density of holes (shown by blue color) is highest at the edges (interface of active region and barriers) of the valence band of the active region even the first heavy holes (heavy
holes associated with first energy state) density is highest at the central region. This figure also shows that the heavy holes density associated with the first energy state is maximum at the central portion; while other heavy holes (i.e. HH2, HH3 etc.) density is higher at the edges of the valence band. In figure 2, the position of the split-off holes band (shown by light blue color) is also shown which lies much below the heavy and light hole bands.

The 4 x 4 Kohn-Luttinger Hamiltonian has been solved to determine the band dispersion (E-K curve) of GaAsP/AlGaAs nano-heterostructure. In figure 2, the dispersion curves for electrons (in conduction band) and holes (i.e. heavy and light holes in valence band) in the quantum well region of the nano-heterostructure Al$_{0.45}$Ga$_{0.55}$As/GaAs$_{0.84}$P$_{0.16}$ are illustrated. Refer figure 2, it is shown that the dispersion curves for the electrons associated with the $E_1$ and $E_2$ energy states within the conduction band of quantum well region of GaAsP layer are almost parabolic in nature. In figure 2, the dispersion profile for holes in valence band (i.e. heavy and light holes) associated with the two energy states (HH1 and LH1) of the barrier region of AlGaAs layer is also shown. From figure 2, it may be noticed that at $K_\parallel$=0, HH1 and LH1 both have different energies, but these energy values become almost same for larger value of the wave vector $K_\parallel$.

![Figure 1](image.png)

*Figure 1.* Picturization of probability densities of the carriers in conduction and valence sub-bands in AlGaAs/GaAsP nano-heterostructure.
7.3 Optical Gain Characteristics of the AlGaAs/GaAsP Heterostructure

In order to calculate the total optical gain of type-I Al$_{0.45}$Ga$_{0.55}$As/GaAs$_{0.84}$P$_{0.16}$ symmetric nano-heterostructure the required parameters are the momentum matrix elements and the transition dipole moments. These parameters are calculated within the framework of HD studio package. Actually, the transition dipole moment gives the information about the phase factors of the two energy states which are responsible for the optical transitions to provide the optical gain of the heterostructure. Moreover, the square of its magnitude tells the interaction strength. In figure 3, the calculated TE and TM optical gain (at 70 K) of type-I Al$_{0.45}$Ga$_{0.55}$As/GaAs$_{0.84}$P$_{0.16}$ symmetric nano-heterostructure is plotted and shown. This figure confirms that the TM optical gain is much greater than that TE gain. This trend of optical gain is opposed to the general trend. In general, the TE optical gain is found greater than TM mode. Refer to figure 3, the maximum TM optical gain is found ~ 5000 /cm giving photonic energy of ~ 1.66 eV and emission wavelength of ~ 0.746 µm; while within the TE mode, the maximum optical gain is found ~ 1174 /cm producing the same photonic energy and same emission wavelength. The overall optical gain of the heterostructure is found within the visible region.
Figure 3. Illustration of optical gain (in TE and TM modes) of AlGaAs/GaAsP nano-heterostructure.

7.4 Effect of Temperature on Optical Gain Characteristics and Wavelength

In order to observe the effect of temperature on the optical gain of the AlGaAs/GaAsP nano-heterostructure, the optical gain was calculated several times for different temperatures ranging from 70 K to 300 K (room temperature). The outcomes of the calculations are plotted in figures 4, 5 and 6. In figures 4 and 5, the variation of TE and TM optical gain, respectively, with temperature for AlGaAs/GaAsP nano-heterostructure is shown. In both the figures, it is shown that the both TE and TM optical gain reduces significantly with increasing the temperature. Obviously, the increasing temperature degrades the optical performance of the heterostructure. The degradation may attributed to the various factors such as broadening of the gain peak, changes in non radiative recombination rates and the increase in losses produced due to higher current densities. The increasing temperature also shows the significant effect on the emission wavelength, as shown in figure 6. The emission wavelength of the heterostructure is found to increase with increase in temperature.
Figure 4. Variation of TE optical gain with temperature for AlGaAs/GaAsP nano-heterostructure.

Figure 5. Variation of TM optical gain with temperature for AlGaAs/GaAsP nano-heterostructure.
Variation in emission wavelength of AlGaAs/GaAsP nano-heterostructure with temperature.

**Figure 6.** Variation in emission wavelength of AlGaAs/GaAsP nano-heterostructure with temperature.

### 7.5 Effects of External Electric Field on Optical Gain Spectra

Before the observation of effect of external electric field on the optical response such as optical gain of the GaAsP/AlGaAs nano-heterostructure, it is important to explore and understanding the physics of the energy band diagram of the GaAsP/AlGaAs nano-heterostructure under study showing the probability density of the associated charge carriers responsible for the transitions producing the desired optical gain and as well as emission wavelength. It is also important to study the E-K dispersion curve of the quantum well region of the heterostructure under the external electric field applied.

Figure 7 shows that how the electrons and holes confined with conduction band and valence band, respectively, of the quantum well region are shifted under the external electric field applied on the GaAsP/AlGaAs nano-heterostructure. Under the electric field applied, the potentials of the electrons and holes are modified according to the mathematical formalism $V = -\int E dx$, where $E$ is the electric field applied and integral is taken over space. Due to the change in potentials of electrons and holes, the associated energy levels are changed and hence the emission wavelength of the heterostructure is changed. These all facts have been studied experimentally and as well as theoretically by E. V. Filatov et al. [2], in
which they have studied the mechanism of type-II ZnSe/BeTe heterostructure under external electric field applied (100 kV/cm).

Figure 8 shows the modified dispersion curve (E-K curve) due to the applied external electric field (electric field~100 KV/cm) on the GaAsP/AlGaAs ano-heterostructure. From this figure the small reduction in energy band gap due to applied external electric field may be noticed, due to which increased optical wavelength may be emitted. The comparative study of figures 2 and 8 confirms that in the dispersion curve (without electric field) the energy values of both holes HH1 and LH1 become almost same for larger value of the wave vector \( K_{||} \); while in the dispersion curve under external applied electric field the energy values of both holes HH1 and LH1 do not approach each other for the same values of the \( K_{||} \) wave vector, as in case of absent of external electric field.

**Figure 7.** Picturization of probability densities of the carriers in conduction and valence sub-bands in AlGaAs/GaAsP nano-heterostructure under external electric field.
Initially, a small electric field (~50 KV/cm) is applied on GaAsP/AlGaAs nano-heterostructure in order to observe the electric field effect of optical gain and optical wavelength emitted from the heterostructure. Figure 9 shows the computed optical gain of the heterostructure under 50 KV/cm electric field applied. The comparative study of figures 3 and 9 shows that on the application of electric field ~ 50 KV/cm on the heterostructure the overall TM optical gain is reduced by an amount of ~ 2200 /cm, and the overall TE optical gain is reduced by an amount of ~ 500 /cm. This is drastic change in the optical gain under the field applied on the heterostructure. Moreover, under the influence of the electric field, the photonic energy emitted from the heterostructure is also shifted towards left hand side i.e. towards longer wavelength limit. The inset picture of figure 9 shows the optical gain (taking into account the spin of electrons and holes) due to transitions between individual electrons and holes having parallel and anti-parallel spins.

For this GaAsP/AlGaAs nano-heterostructure, the important observation is that the TM optical gain is greater than TE optical gain; while there are several examples of the heterostructures which have exhibited the greater TE optical gain than TM optical gain [3-5].
This is because of larger relative transition strength of the transitions between conduction band electrons and valence sub-band light-holes (CB-LH) in TM mode rather than the transitions between conduction band electrons and valence sub-band heavy-holes (CB-HH) in TE mode. Since for the GaAsP/AlGaAs nano-heterostructure, the TM mode gain is greater than TE mode, hence TM mode is calculated under different values of external electric field. The significant change in optical gain and emitted photonic energy under different values of electric field on the heterostructure is shown in figure 10. Further, the reducing optical gain within TM mode and increasing optical wavelength with increasing magnitude of applied electric field is summarized in figure 11 (a) and (b). The reason behind the increasing wavelength with increasing electric field is that the electronic states are shifted downwards, while the holes states are shifted to upwards which results into reduction of frequencies and hence increasing the optical wavelength.

Figure 9. Illustration of optical gain (in TE and TM modes) of GaAsP /AlGaAs nano-heterostructure under applied electric field ~ 50 KV/cm.
Figure 10. Illustration of total TM optical gain of GaAsP /AlGaAs nano-heterostructure under different values of applied external electric field.

Figure 11. Variation of (a) peak optical gain with in TM mode (b) emission wavelength with applied external electric field on GaAsP /AlGaAs nano-heterostructure.

7.6 Uniaxial Strain Effects on Optical Gain Spectra

In figures 12, 13 and 14, the uniaxial strain effects on optical gain spectra and emitted wavelength of GaAsP/AlGaAs nano-heterostructure are shown. The uniaxial strain is applied along [100] direction. In figure 12, it is shown that the TE optical gain decreases with increasing uniaxial strain ranging from 1 GPa to 15 GPa. Similarly, the TM optical gain is
also found to decrease with increasing uniaxial strain along [100] direction, as shown in figure 13. But the rate of change of TE gain is found different from the rate of change of TM gain. The optical wavelength emitted from the heterostructure is also found to shift towards higher region. In figure 14, it is shown that increasing order of uniaxial [100] strain shifts the wavelength towards the longer region. All these facts show the tunability of the GaAsP/AlGaAs nano-heterostructures under variable uniaxial strain. The results are coherent with the results obtained for the InGaAlAs/InP nano-heterostructure under different types of strains [6].

Figure 12. Variation of TE optical gain with uniaxial strain along [100] direction.
**Figure 13.** Variation of TM optical gain with uniaxial strain along [100] direction.

**Figure 14.** Effect of uniaxial [100] strain on emission wavelength for GaAsP/AlGaAs nano-heterostructure.

**References**


3. P. A. Alvi, Pyare Lal, S. Dalela, M. J. Siddiqui, "An Extensive Study on Simple and GRIN SCH based In_{0.71}Ga_{0.21}Al_{0.08}As/InP Lasing heterostructure", Physica Scripta, 85, 035402 (2012).

