InGaAsN/GaAs TYPE-I NANO-SCALE HETEROSTRUCTURE

Recently, the quaternary material InGaAsN has drawn considerable attention as compared to the other quaternary materials such as InGaAlAs, InGaAsP, and InGaAlP; because the addition of a small nitrogen (N) fraction compensates the compressive strain that limits the critical thickness of GaInAs layers grown on GaAs substrates. The InGaAsN alloy may be considered to be made of \((\text{GaAs})_{1-z} (\text{InAs}_{0.62}\text{N}_{0.38})_z\), but in this work it has been to have combination of two ternaries i.e. combination of GaAsN and InAsN ternary alloys. Moreover, InGaAsN quaternary material based heterostructures with very low nitrogen concentrations (with diluted N) have came recently into consideration due to the band gap variation in negative way, (i.e. the reduction of the band gap with addition of nitrogen). Thus, the heterostructures having N-containing III-V semiconductor alloys GaAsN and InGaAsN have grown fundamental and commercial interest; and therefore, this chapter has a detailed study directed towards modeling and designing of \(\text{In}_{0.29}\text{Ga}_{0.71}\text{As}_{0.99}\text{N}_{0.01}/\text{GaAs}\) nanoscale-heterostructure having a single QW of thickness \(\sim 60\) Å and optimization of optical characteristics such as optical and mode gain, differential gain, gain compression, anti-guiding factor, transparency wavelength, relaxation oscillation frequency (ROF), optical power and their mutual variation behavior.

8.1 Design Parameters of InGaAsN/GaAs Heterostructure

The proposed heterostructure InGaAsN/GaAs has been considered to have a sandwich structure, consisting of an active region of single quantum well of \(\text{In}_{0.29}\text{Ga}_{0.71}\text{As}_{0.99}\text{N}_{0.01}\) in between the barrier layers of GaAsN followed by claddings layers of GaAsN. The well or active region is of the order of \(\sim 60\) Å, barrier region \(\sim 50\) Å, while cladding \(\sim 100\) Å. Thus the entire structure is sized as \(\sim 21\) nm and hence the name is nano-heterostructure. The region behind the chosen of such size of active region is to have quantum confinement of the envelope function (or wave function) associated with the quantum well. Because, for the quantum mechanical observations such as optical emission or optical absorption, the size of the active region should be comparable to the de-Broglie wavelength. The entire structure is supposed to be grown over GaAs substrate. This substrate is selected due to its lattice parameters which are matched with active region...
parameters of the structure. The lattice matching of active region material with the substrate is very important otherwise strain is produced which may degrade the device performance. For example, in a recent work, type-I InGaAs/GaAsP nano-heterostructure gown pseudomorphically on GaAs substrate (in which InGaAs material is lattice matched with GaAs substrate) has been found to exhibit good performance [1]. This is STIN (Step-Index) heterostructure because refractive index of quantum well region abruptly changes at the interface of barrier and well region. Its complete design parameters related to its energy band diagram are listed in table 1.

<table>
<thead>
<tr>
<th>Role of Layer</th>
<th>Layers Specification</th>
<th>Layers Thickness (Å)</th>
<th>Lattice constants (Å)</th>
<th>Strain</th>
<th>Conduction band edge-offset (eV)</th>
<th>Valence band edge-offset (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantum well</td>
<td>In$<em>{0.29}$Ga$</em>{0.71}$As$<em>{0.99}$N$</em>{0.01}$</td>
<td>60</td>
<td>5.766</td>
<td>-0.020</td>
<td>0.1076888</td>
<td>-0.0538444</td>
</tr>
<tr>
<td>Barrier</td>
<td>GaAs$<em>{0.10}$N$</em>{0.90}$</td>
<td>50</td>
<td>6.017</td>
<td>-0.060</td>
<td>0.3450696</td>
<td>-0.1478870</td>
</tr>
<tr>
<td>Cladding</td>
<td>GaAs$<em>{0.41}$N$</em>{0.59}$</td>
<td>100</td>
<td>5.892</td>
<td>-0.040</td>
<td>0.7036184</td>
<td>-0.3015508</td>
</tr>
<tr>
<td>Substrate</td>
<td>GaAs</td>
<td>-</td>
<td>5.653</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

8.2 Computation of Wavefunctions and Discrete Energies

For the computations of wavefunctions and energies of conduction and valence subbands (heavy and light holes) of InGaAsN QW heterostructure, \( \mathbf{k}.\mathbf{p} \) method has been utilized along with effective mass approximation. The calculated wavefunctions associated with electrons and holes are not being shown here. The calculated discrete energies of conduction band electrons and valence band holes are shown below:

**CONDUCTION BAND ELECTRON ENERGIES**

Energy of first electronic state: 0.178 eV
Energy of second electronic state: 0.349 eV
Energy of third electronic state: 0.451 eV
Energy of fourth electronic state: 0.529 eV
Energy of fifth electronic state: 0.690 eV
VALENCE SUBBAND ENERGIES

For Heavy Holes (HH)

Energy of first hole (HH) state: 0.867 eV
Energy of second hole (HH) state: -0.122 eV
Energy of third hole (HH) state: -0.167 eV
Energy of fourth hole (HH) state: -0.178 eV
Energy of fifth hole (HH) state: -0.218 eV
Energy of sixth hole (HH) state: -0.252 eV

For Light Holes (LH)

Energy of first hole (LH) state: -0.150 eV
Energy of second hole (LH) state: -0.190 eV
Energy of third hole (LH) state: -0.240 eV
Energy of fourth hole (LH) state: -0.297 eV

Thus, there are five conduction band electrons, six heavy holes and four light holes are responsible for optical processes. But dominant transition takes place between e1 (first conduction band electron) and HH1 (first heavy holes) and LH1 (first light hole). From the above data, it is clear that first heavy hole (HH1) is found to lie above the first light hole (LH1). This condition confirms that the designed InGaAsN QW heterostructure is a strained (compressive strain) heterostructure as shown in figure 1.

![Figure 1](image_url)

**Figure 1.** Representation of energy band structure (E-K curve) under different states of strain [2].
8.3 Study of quasi-Fermi levels

The study of quasi Fermi levels is essential requirement to explain the behavior of optical gain in the QW Straddled type heterostructures. The separation between quasi Fermi energy levels plays a critical role in the semiconducting heterostructure because of its relationship with the density of injected carriers and the intensity of optical gain [3]. In figures 2 and 3, the behavior of quasi Fermi levels for electrons in the conduction and holes in the valence bands, respectively, is shown for In$_{0.29}$Ga$_{0.71}$As$_{0.99}$N$_{0.01}$/GaAs straddled heterostructure. Figure 2 and 3 predicts that quasi Fermi energies for both the conduction and valence bands are increased as increase in carrier density. Further, on merging the figure 2 and 3 simultaneously, it can be observed that the separation between both the quasi Fermi levels is also increase as increase in carrier densities. Thus, this separation has crucial role in the existence of optical gain in the designed In$_{0.29}$Ga$_{0.71}$As$_{0.99}$N$_{0.01}$/GaAs straddled heterostructures. In order to achieve the optical gain in the designed heterostructure, the separation between the quasi Fermi levels must be greater than the energy band gap of the material of the quantum well within the heterostructure; otherwise optical gain will not exist. This means that for existing the optical gain in the designed heterostructure, the required condition is $(F_c-F_v) > E_g$.

![Behavior of Quasi-Fermi Level in conduction band](image)

**Figure 2.** Representation of conduction band quasi-Fermi energy for InGaAsN QW heterostructure.
8.4 Gain Spectra of In0.29Ga0.71As0.99N0.01/GaAs straddled heterostructure

The most important and basic characteristic of the optoelectronic-devices considering heterostructures is the Optical Gain whose study is required for the realization of a semiconductor laser like optoelectronic-devices because it describes the optical amplification in the semiconductor material. Actually, the optical gain occurs due to the stimulated emission taking place by recombination of conduction band electrons and valence band holes. According to the theory of density matrix, the optical gain can be determined by summing up contribution from overall transitions in between the electrons and holes in the conduction and valence subbands, respectively. Again, another important basic characteristic is the modal gain which depends on the confinement factor, GRIN (graded refractive index) layers, number of quantum wells and device geometry; hence understanding of modal gain is a major objective as being a basic requirement for device optimization [4]. For In0.29Ga0.71As0.99N0.01/GaAs straddled heterostructure, the behaviors of optical gain and modal gain in terms of lasing wavelength are simultaneously plotted in figure 4 for carrier concentrations of (~2×10^{18} cm^{-3}). In the both spectra of optical gain and modal gain, two peaks are observed. Occurring of the upper peak is due to transition between electrons associated with first conduction subband and first heavy hole.
valence subband; while the lower peak is obtained due to transition between first conduction subband electrons and first light hole valence subband.

![Optical Gain and Modal Gain with Lasing Wavelength](image)

**Figure 4.** Optical gain and modal gain as a function of wavelength for In$_{0.29}$Ga$_{0.71}$As$_{0.99}$N$_{0.01}$/GaAs straddled heterostructure

In figure 4, it can be observed that the maximum optical gain and modal gain is obtained of the order of ~2100 cm$^{-1}$ and 20 cm$^{-1}$, respectively, at lasing wavelength of 1.30 µm. Actually, the lasing heterostructures emitting the radiations in the wavelengths ~ 1.3 µm have generated great interest for applications in optical fiber communications because the 1.3 µm wavelength is attractive due to zero dispersion in the silica based optical fiber.

The results obtained for type-I InGaAsN/GaAs heterostructure have also been compared with the optical gain of type-I InGaAlAs/InP nano-heterostructure having the same geometry and shown in figure 5. From figure 5, it is clear that for the InGaAsN/GaAs heterostructure, the obtained maximum optical gain (i.e. ~2100 cm$^{-1}$ at 1.30 micrometer) is almost half of the maximum optical gain (i.e. ~4200 cm$^{-1}$ at 1.55 micrometer) of InGaAlAs/InP straddled heterostructure. In addition, the non linear behavior of peak modal gain and peak optical gain with current density for In$_{0.29}$Ga$_{0.71}$As$_{0.99}$N$_{0.01}$/GaAs straddled heterostructures is also shown in figure 6. In figure 6, it can be seen that for any value of current density the obtained peak optical gain is approximately more than hundred times of peak modal gain.
Figure 5. Comparison of optical gain for InGaAlAs/InP and InGaAsN/GaAs straddled heterostructure

Figure 6. Peak modal gain and peak optical gain with current density for In$_{0.29}$Ga$_{0.71}$As$_{0.99}$N$_{0.01}$/GaAs straddled heterostructure
The study of spectrum of refractive index of QWs in the heterostructure has vital role in the design and implementation of nano-scale opto-electronic equipments. In literature, it has been reported that a quantum-well laser have a higher gain and a smaller refractive-index change than a conventional diode laser [5]. For heterostructure, the most important differences between the quantum well or active region and barrier layers occur normally in the energy of band-gap and the index of refraction. Refractive index change and peak optical gain with carrier density for In$_{0.29}$Ga$_{0.71}$As$_{0.99}$N$_{0.01}$/GaAs straddled heterostructure are plotted on right and left y-axes, respectively, in figure 7. In the lower carrier density regime, figure 7 shows that the refractive index change and peak optical gain exhibit inversely behavior with carrier density, while for higher carrier density region both the refractive index change and peak optical gain exhibit proportional behavior with carrier density.

![Graph](image)

**Figure 7.** Peak optical gain and refractive index change gain with carrier density for In$_{0.29}$Ga$_{0.71}$As$_{0.99}$N$_{0.01}$/GaAs straddled heterostructure.

For In$_{0.29}$Ga$_{0.71}$As$_{0.99}$N$_{0.01}$/GaAs straddled heterostructure, the differential gain (first derivative of optical gain with respect to carrier density) and gain compression (gain saturation or non linear gain coefficient) have also been studied and plotted in figures 8 and 9, respectively. The gain compression factor is substantial parameter to design properly QW lasing structures. This factor can also be used in shaping the amplitude and frequency modulation of the lasing diodes. In general, the linear gain does not dependent of the density of photon. However, at upper photonic
densities, the gain tends to reduce; this reduction behavior of gain is termed as gain compression. The gain compression is basically caused by the depletion of electrons at fixed energy levels due to strong stimulated recombination or spectral holes burning. Again from figures 8 and 9, it is clear that both differential gain and gain compression vary in proportional way with varying carrier density.

**Figure 8.** Differential gain with Carrier density for In$_{0.29}$Ga$_{0.71}$As$_{0.99}$N$_{0.01}$/GaAs straddled heterostructure

**Figure 9.** Gain compression with Carrier density for In$_{0.29}$Ga$_{0.71}$As$_{0.99}$N$_{0.01}$/GaAs straddled heterostructure
8.5 Anti-guiding factor of In$_{0.29}$Ga$_{0.71}$As$_{0.99}$N$_{0.01}$/GaAs straddled heterostructure

In addition to the optical gain, and differential gain, the anti-guiding factor is also a substantial and responsible parameter for the dynamics performance of quantum well heterostructures based lasers. The anti-guiding factor plays a very crucial role in deciding the optical gain of lasing heterostructure and can be defined in terms of refractive index change and differential gain. The anti-guiding factor has been calculated with the help of formula: \( \alpha = 4\pi(-n')/\lambda G \); where \( G \) is the differential gain, \( n' \) is the differential refractive index change with respect to carrier concentration and \( \lambda \) is the lasing wavelength. For the In$_{0.29}$Ga$_{0.71}$As$_{0.99}$N$_{0.01}$/GaAs straddled heterostructure, the behavior of anti-guiding factor has been plotted in figure 10. From figure 10, it is clear that the range of anti-guiding factor is found to vary from 1.4 to 2.4. Here, it is important to note the smaller value of anti-guiding factor is more desirable. In literature, smaller values have been predicted and reported for doped/strained and quantum-well (QW) heterostructures [6-9]. Actually, the anti-guiding factor supports the optical gain because both have proportional behavior with carrier density. The proportional behavior of anti-guiding factor and peak optical gain with carrier density for In$_{0.29}$Ga$_{0.71}$As$_{0.99}$N$_{0.01}$/GaAs straddled heterostructures are shown in figure 11.

![Figure 10. Behavior of Anti-Guiding factor with Carrier density for In$_{0.29}$Ga$_{0.71}$As$_{0.99}$N$_{0.01}$/GaAs straddled heterostructure.](image)
Figure 11. Anti-guiding factor and Peak Optical gain with Carrier density for In$_{0.29}$Ga$_{0.71}$As$_{0.99}$N$_{0.01}$/GaAs straddled heterostructure.

8.6 Leakage Current Density, Relaxation Oscillation Frequency and Optical Output Power

For In$_{0.29}$Ga$_{0.71}$As$_{0.99}$N$_{0.01}$/GaAs material system based lasing heterostructure, the behavior of leakage current has also been studied and plotted in figure 12. From figure it can be seen that the leakage current approximately remains same at low value of carrier density, while at higher value of carrier density it increases drastically. Next, relaxation oscillation frequency (ROF) and optical output power have important role in the determination of threshold current. The fixed value of current at which relaxation oscillation frequency and optical output power both are obtained negligible is called threshold current. Basically, above the threshold current the optical gain occurs positive while below the threshold current it becomes negative. The relaxation oscillation frequency and optical output power with current for In$_{0.29}$Ga$_{0.71}$As$_{0.99}$N$_{0.01}$/GaAs straddled heterostructures are plotted on left and right y-axes, respectively, in figure 13. Figure 13 shows that the optical output power and relaxation oscillation frequency do not exist at current ~ 100 mA (threshold current). It is clear by curves of figure 13 that above the threshold current, the optical output power and relaxation oscillation frequency both are enhanced with the increase in current.
Figure 12. Leakage current density with carrier density for In$_{0.29}$Ga$_{0.71}$As$_{0.99}$N$_{0.01}$/GaAs straddled heterostructures

Figure 13. Relaxation oscillation frequency and optical output power with current In$_{0.29}$Ga$_{0.71}$As$_{0.99}$N$_{0.01}$/GaAs straddled heterostructures
References

1. H. K. Nirmal, S. G. Anjum, Pyare Lal, Amit Rathi, S. Dalela, M. J. Siddiqui, P. A. Alvi, “Field effective band alignment and optical gain in type-I Al\(_{0.45}\)Ga\(_{0.55}\)As/GaAs\(_{0.84}\)P\(_{0.16}\) nano-heterostructures”, Optik 127, pp. 7274–7282 (2016).


