Analysis of properties of nitride based quantum well laser diode using Luttinger-Kohn hamiltonian

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The paper presents the analyses of the influence of carrier concentration and applied voltage on the various optical and electrical characteristics. The analyses have been carried out through Luttinger-Kohn Hamiltonian and the Schrodinger and Poisson's equations have been solved in a self-consistent manner. The effects of strain and piezoelectric polarization on quantum well laser diode are included in the analyses. We have achieved better optical gain and quantum efficiency for single quantum well lasers.

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1. Introduction

Quantum Well Lasers are a class of semiconductor lasers that have ultra thin active layers forming narrow potential wells for injected carriers and giving rise to a size quantization of the electronic status. Today, researchers in quantum optics are interested in the physics of semiconductor lasers, which have cavity comparable to wavelengths and to improve laser characteristics by miniaturizing device structures. Light emitters such as light-emitting diodes (LEDs) and laser diodes convert electrical energy into optical energy [1]. The development of light sources which emit only the desired part of the spectrum with higher efficiency and a longer lifetime than incandescent bulbs are very lucrative venture. III–V nitride semiconductors provide the materials basis for a number of well-established commercial technologies, as well as new cutting-edge classes of electronic and optoelectronic devices. Hence, the emphasis has been given on III-V Nitride laser diodes [2-3].

Furthermore, developing large applications is a complex process, particularly to carry out trail and error method in fabrication is too expensive. Therefore, the assistance of adequate programming tools is always welcome. Not surprisingly, there are numerous commercially available tools for this purpose. Performance tuning, debugging and data analysis are more difficult, and yet tools that are simultaneously sustainable, highly functional, robust and easy to use for quantum structure based laser diode analysis are not widely available. This is partially due to the difficulty of developing sophisticated and customized simulation tools. Therefore, it is necessary to develop the computer simulation tools which fulfil these conditions. The simulation tools have the advantage to reduce the cost of prototyping of semiconductor lasers and provide a better insight of device properties to the analyst prior to fabricating an actual device. Hence, the paper has been focussed on the theoretical investigation of optical and electrical characteristics of single quantum well lasers. The paper is being divided in three sections; second section of the paper presents the mathematical approach. While, the third section reveals the detail discussion of the obtained results, followed by a conclusions.

2. Theoretical explanations

The quantization effect paramount with miniaturization and hence it is necessary to analyze the quantum structures using quantum mechanics rather than classical theory. To analyze the quantization effect in quantum structure the Schrödinger equation has been solved by using Transfer matrix method [4]. Where, the time independent Schrödinger equation is given as follows

$$-\frac{h}{4m^{*}\pi}\frac{\partial^{2}\psi(z)}{\partial z^{2}}+V(z)\psi(z)=E\,\psi(z) \qquad (1)$$

here, m^* is the effective mass, h is the Planck's constant and E is the Eigen energy. The Poisson equation is given as,

$$\frac{\partial^{2}\phi(Z)}{\partial Z^{2}}=-\frac{1}{\varepsilon}\left(Q_h+Q_e+Q_{pz}\right) \qquad (2)$$

where, $\phi(z)$ is the solution of the Poisson equation with strained induced electric field, Q_e, Q_h, and Q_{pz}, are the charge density of electrons, hole and the piezoelectric respectively and ε is the dielectric constant of the material.

The electronic properties can be analyzed through various theoretical approaches such as Airy's function, variational method, quasi transmitting boundary method, transfer matrix method, k. p. method, Pseudo potential theory etc [5-7]. The k.p. Model predicts band structure and effective mass for electrons and holes in a semiconductor as a result of the periodic potential. The model approximates the actual electrostatic potential of quantum well structures and by means of a perturbative approach, it provides a continuation in the wave vector k

of the energy bands in the vicinity of some special point in the Brillouin zone (BZ). In the analyses of conventional III-V nitride semiconductors 4 X 4 and 6 X 6 Luttinger-Kohn Hamiltonians [8-11] are used. Here, the Luttinger Kohn Hamiltonian of 4 X 4 k. p. model is denoted by H and given in equation (3),

$$H=\begin{bmatrix} -(P+Q) & S & -R & 0 \\ -S^{*} & -P+Q & 0 & -R \\ R^{*} & P-Q & -P+Q & -S \\ 0 & R^{*} & S^{*} & -(P+Q) \end{bmatrix} \begin{matrix} \left|\frac{3}{2},\frac{3}{2}\right\rangle \\ \left|\frac{3}{2},\frac{1}{2}\right\rangle \\ \left|\frac{3}{2},\frac{-1}{2}\right\rangle \\ \left|\frac{3}{2},\frac{-3}{2}\right\rangle \end{matrix} \quad (3)$$

In the above expression P, Q, R, and S are the matrix elements given by the following relations. The Eigen values and eigenvector of the 4 X 4 Luttinger-Kohn Hamiltonian then used in the solution of the Schrödinger equation to analyze the electron/hole transport phenomena in the quantum well structure. At this point the matrix element of 4 X 4 Hamiltonian is given equation (4),

$$P = \frac{h^2}{4\pi m_0}\gamma_1\left(k_x^2 + k_y^2 + k_z^2\right) \quad (4a)$$

$$Q = \frac{h^2}{4\pi m_0}\gamma_2\left(k_x^2 + k_y^2 - 2k_z^2\right) \quad (4b)$$

$$R = \frac{h^2}{4\pi m_0}\sqrt{3}\left[-\gamma_2\left(k_x^2 - k_y^2\right) + 2i\gamma_3 k_x k_y\right] \quad (4c)$$

$$S = \frac{h^2}{4\pi m_0} 2\sqrt{3}\gamma_3\left(k_x - ik_y\right)k_z \quad (4d)$$

The variables γ_1, γ_2 and γ_3 are the Luttinger parameters [12] which are the functions of the lattice parameters and hence includes the strain effect. The basis set of the Luttinger-Kohn Hamiltonian in linear combinations along with the spin can be represented in the following Table 1.

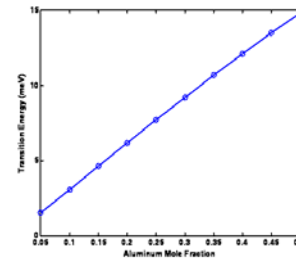
Table 1. Basis function in Luttinger-Kohn Hamiltonian

u_i	$\left\|J, J_Z\right\rangle$	$\psi_{J,Jz}$
u_1	$\left\|\frac{3}{2},\frac{3}{2}\right\rangle$	$\frac{1}{\sqrt{2}}\left\|(X+iY)\uparrow\right\rangle$
u_2	$\left\|\frac{3}{2},\frac{1}{2}\right\rangle$	$-\sqrt{\frac{2}{3}}\left\|Z\uparrow\right\rangle+\frac{1}{\sqrt{6}}\left\|(X+iY)\downarrow\right\rangle$
u_3	$\left\|\frac{3}{2},\frac{-1}{2}\right\rangle$	$\frac{1}{\sqrt{6}}\left\|(X-iY)\uparrow\right\rangle+\sqrt{\frac{2}{3}}\left\|Z\downarrow\right\rangle$
u_4	$\left\|\frac{3}{2},\frac{-3}{2}\right\rangle$	$\frac{1}{\sqrt{2}}\left\|(X-iY)\downarrow\right\rangle$

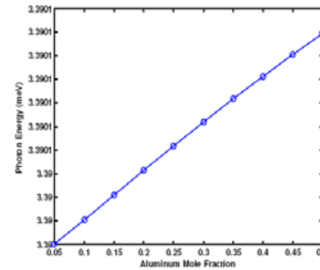
The self consistent solution have been utilized to obtained the recombination rate [13], optical gain [14], internal loss, carrier concentration and quantum efficiency [15], these results are discussed in the section III.

3. Results and discussion

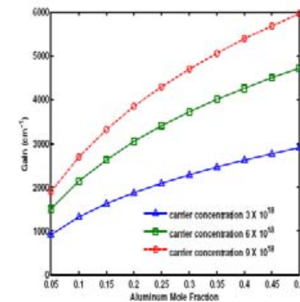
The optical gain coefficient is one of the crucial indicators of a semiconductor material's quality for laser applications. An increase in Aluminium mole, increases the potential depth of the quantum well which results in enhancement of photon energy and the transition energy as revealed in Fig. 1 a and b. Hence, the optical gain is observed to be increasing as shown in Fig 1c with the increase in the Aluminium mole fraction due to the increase in the photon and transition energies. The increase in the mole fraction results the incorporation of a heavier electron and holes in the cladding layer (AlGaN) and significantly affects to Fermi energy levels of conduction and valance band states. As it is obvious with increase in the Al concentration, recombination rate is enhanced and so the optical gain is achieved more for the higher Al concentration for all density of states.



(a)



(b)



(c)

Fig. 1 (a) Transition energy as a function of Al mole fraction;(b) Photon energy as a function of Al mole fraction; (c) Optical gain as a function of Al mole fraction.

Fig. 2 reveals the recombination rate in quantum well laser for different effective density of state 2.3 x 10^{18} cm^{-3}. The recombination rate has been determined by k.p. method, with the inclusion of strained effect through Luttinger parameters. The variation of recombination rate has been calculated for valance band density of states Nv =2.3 X 10^{17} cm^{-3} with quantum well width 5nm at 30% Aluminum mole fraction. It has been observed recombination at the centre of the device reaches to its peak value which is found to be 13.65937 X 10^{26} cm^{-3}. The results obtained through developed simulation tools shows a good agreement with results as reported by J. Piprek et.al [16]. It is realized during analysis that with increase in the conduction band density of states, there is a nonlinear decrease in the recombination rate.

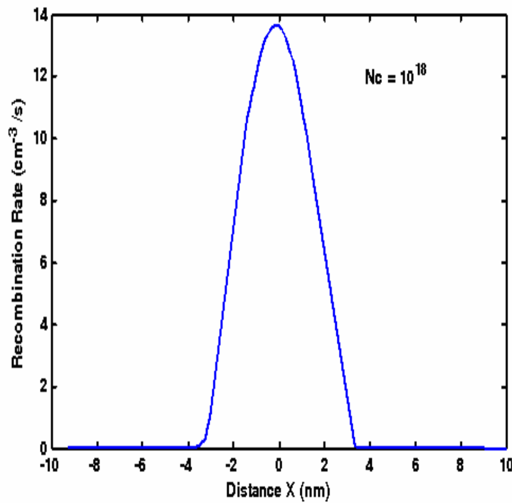


Fig. 2 Recombination rate (10^{26}) along distance X single quantum well laser.

One of the crucial parameter in device performance analysis is the carrier concentration which is involved in the determination of threshold current density and other parameters. Fig. 3 shows the variation of carrier concentration along X-axis and Y-axis of the quantum well laser diode. The carrier concentration has been obtained from self-consistent solution, the result have been obtained for 30% mole fraction of Aluminum in $Al_xGa_{1-x}N$ and well width of 5 nm. From the result it is revealed that the maximum carrier concentration is achieved in the centre of the symmetric single quantum well structure. Further, it has been observed that maximum concentration is obtained for 6 Volt of biasing and the value of this maximum carrier concentration is 2.7*10^{19} for 6 Volt, during investigation of bias voltage variation it was observed that the change in maximum carrier concentration for 6volt to 3 Volt the carrier concentration reduces by 3.1*10^{9}. The decrease in carrier concentration is attributed to the decrease in the Eigen energy E which affects wavevector of the barrier region and well region both. At higher voltage well region has the maximum concentration which is faceted due to the shrink [17] in the bandgap energy which affects the band offset between the barrier region and well region. The increase in applied bias causes the concentration escalation in the well region, due to upset in the steady-state balance between drift and diffusion, which unleashes the flow of diffusion current.

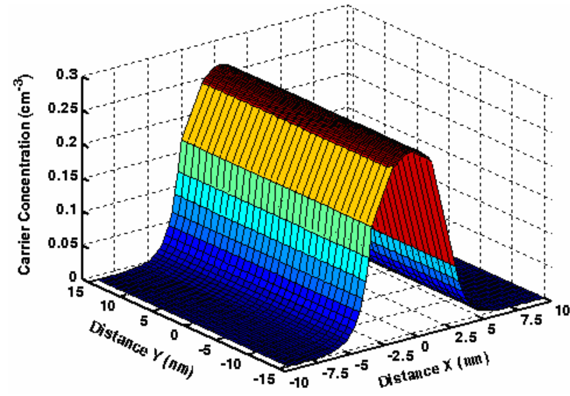


Fig. 3 Electron concentration distribution (10^{19}) in single quantum well for 6volt.

The quantum efficiency is one of the key performance parameters of laser diodes. The analysis of quantum efficiency has been carried out along with the internal losses of the quantum well laser diode. The internal loss is the function of the confinement factor estimated as

$$\alpha_{th} = \alpha_{sc} + \alpha_{fca}\Gamma_w + \alpha_{wg}(1-\Gamma_w) + \frac{\log(1/R)}{L}$$

where, α_{sc} is scattering losses, α_{fca} is free carrier absorption, Γ_w is the optical confinement factor, α_{wg} is the waveguide loss and L is the cavity length. Figs. 4 to 5 show the internal losses and quantum efficiency variation with Aluminium mole fraction.

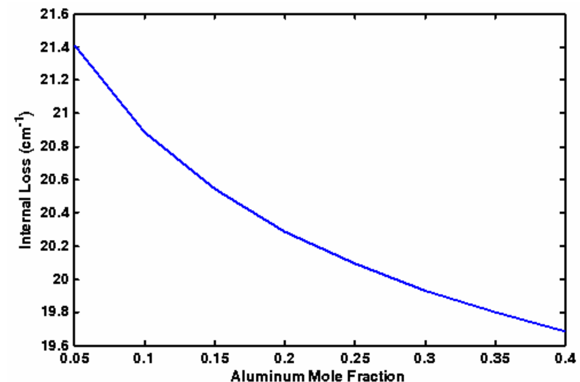


Fig. 4 Internal loss variation as a function of Aluminium mole fraction.

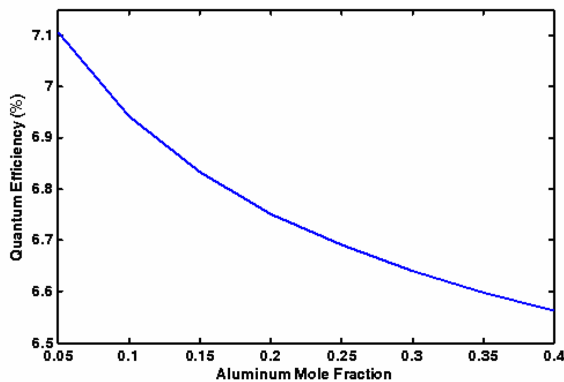


Fig. 5 Quantum efficiency variation with Aluminium mole fraction.

The lowering of the internal loss with the increasing Aluminium concentration has been observed in our analysis as shown in Fig. 4. Further the increase in the mole fraction of the Aluminum in $Al_xGa_{1-x}N$ increases the step index between the well and the claddings which reduces the internal losses. The quantum efficiency for varying Aluminum mole fraction has been depicted in Fig. 5. Here, the quantum well width was taken to be 5 nm while the wavelength used in calculation over is 375nm.

4. Conclusions

The efforts have been made to optimise the physical and material properties to achieve reduction in carrier losses to minimize self-heating and achieve higher output power. It has been concluded that quantum confinement and piezoelectric field allows one to fine-tune the energy and strength of optical transitions in GaN quantum well laser diodes by smart choice of band offset and well width. We have achieved better quantum efficiency, optical gain and higher recombination rate for single quantum well laser diode.

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