Investigation of Diverse Characteristics of Strained III-V Nitride Quantum Well

Edmund P Samuel, Ulhas Sonawane, Bhavana N. Joshi, D. S. Patil

***Abstract*—Maxwell equations in isotropic, dielectric medium have been used to analyze the optical field intensity. Effective index method have been employed to analyze the optical field intensity, the study has been extended to realize Confinement factor dependence on various parameters. A self consistent solution of Schrodinger-Poisson equation were used to obtain carrier concentration. Piezoelectric effect occurs due to strained GaN/$Al_xGa_{1-x}N$ have been included in a self-consistent solutions. The dependence of quantum efficiency on Aluminium mole fraction and quantum well width has been investigated.**

***Index Terms*—Schrodinger Equation, Self-consistent, Quantum Well**

I. Introduction

The rapid development in fields such as optical communication engineering, optical computing and optical integrated circuits (OICs) have expanded the interest and increased expectations towards shorter wavelength [1-3] laser diodes. The efficient laser diode requires the higher electron confinement, lower power consumption, lower threshold current density, better recombination rate, higher optical gain etc. which is fulfilled through quantum structures such as single quantum well, multiple quantum well and quantum dot laser diodes. Typical heterostructured single quantum well is shown in the following Fig. 1.

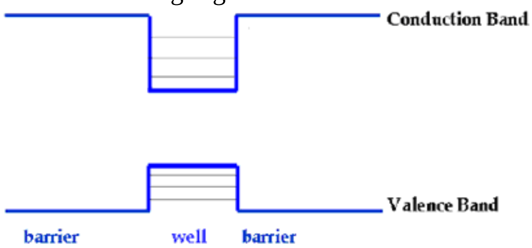

Figure 1 III-V Nitride Single Quantum Well Schematic Structure

Recently, there is a growing interest in improving laser characteristics by miniaturizing device structures. Researchers in quantum optics are interested in the physics of semiconductor lasers, which have cavity comparable to wavelengths. In this paper, we have discussed most important issues needed for the comprehension of light emitters in a proficient form. The emphasis has been given on III-V Nitride laser diodes [4], since they have large bandgap energies necessary for light emission in the wide range of the optical spectrum (green-to-ultraviolet). At present, III–V compound 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. This paper presents a better understanding of device performance characteristics, for the analysis we have developed the composite laser simulation tools. The development of simulation tools has been carried out by using various methods such as quasi transmitting boundary method and transfer matrix method for achieving the solutions from the Schrödinger equations [5-7] and k.p method [8-10] has been used to solve the Schrödinger and Poisson equation self-consistently. The optical analysis has been carried out by solving the Maxwell equations using the effective index method. The paper includes three sections; in section second a mathematical approach is being given. While, section three presents a detail analysis of the results which follows concluding remarks.

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II. Theoretical Elucidation

Numerical computing is a powerful tool for solving multifarious mathematical problems. Developing large applications for a complex process and the assistance of adequate programming tools is always welcome to improve performance tuning, debugging and data analysis. The semiconductor quantum well laser diode very efficiently confines the carriers within the quantum well region, but the optical confinement gets weakened with the reduction in the active region thickness. Hence, to obtain better optical confinement within the quantum well region one needs to optimize the waveguide parameters of the quantum well structure. Maxwell equations in isotropic, dielectric medium have been used to analyze the optical field intensity behavior within the quantum well laser diodes [11-13]. The Maxwell curl equations for these isotropic dielectric materials are solved, in case of transeverse electric (TE) mode, the second order differential equation of electric field component is given in equation (1).

$$\frac{\partial^2 E_y}{\partial^2 x^2} + \left(k_0^2 n^2 - \beta^2\right) E_y = 0 \qquad (1)$$

where, n is refractive index, k_0 is plane wave propagation constant in normal direction, while β is the product of wave propagation constant and effective index. Thus, the general solutions of the field for TE mode are obtained to be as follows,

$$E_y = E_{uc} \exp\left(-\gamma_c x\right) \qquad x>0 \quad \text{(in upper clad)} \qquad (2a)$$

$$E_y = E_f \cos(k_x x + \phi) \quad -T<x<0 \text{ (in well region)} \quad (2b)$$

$$E_y = E_{lc} \exp(\gamma_{lc}(x+T)) \quad x<-T \quad \text{(in lower clad)} \quad (2c)$$

where the wave propagation constants in x direction, expressed in terms of the index N, and are given as,

$$\left.\begin{aligned} \gamma_{uc} &= \sqrt{k_0^2\left(N^2 - n_{uc}^2\right)} \\ k_x &= \sqrt{k_0^2\left(n_f^2 - N^2\right)} \\ \gamma_{lc} &= \sqrt{k_0^2\left(N^2 - n_{lc}^2\right)} \end{aligned}\right\} \quad (3)$$

The near field analysis has been carried out using the above equations to realize the optical field intensity spread in quantum well laser diode.

The optical confinement is achieved in quantum structure is good, but with miniaturization the electron confinement capability of the heterostructure reduces. Hence, it was necessary to optimize the physical and material parameters to achieve better optical and electrical confinement within the quantum well regions. To achieve this self-consistent solution of Schrodinger and Poisson equation has been carried out. The mathematical approach to solve Schrodinger equation have been discussed in, to analyze the quantization effect in quantum structure the Schrödinger equation (4) has been solved by finite difference method.

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

Where, m^* is the effective mass

h, is the Planck's constant,

E, is the Eigen energy and

$$V(z) = -|e|\phi(z) + V_c(z) + |e|Fz \quad (5)$$

At this juncture, e is the electron charge, V_c is the square well potentials for the conduction band, F is the applied electric field, here, ϕ is assumed to be zero for initial calculations. The Poisson equation is

$$\frac{\partial^2\phi(Z)}{\partial Z^2} = -\frac{1}{\varepsilon}\left(Q_h + Q_e + Q_{pz}\right) \quad (6)$$

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 analyses of conventional III-V nitride semiconductors usually use 4 X 4 and 6 X 6 Luttinger-Kohn Hamiltonians [14-15]. Here, the Luttinger Kohn Hamiltonian of 4 X 4 k. p. model is denoted by H and given as follows,

$$H = \begin{bmatrix} -(P+Q) & S & -R & 0 \\ -S^* & -P+Q & 0 & -R \\ R^* & P-Q & -P+Q & -S \\ 0 & R^* & S^* & -(P+Q) \end{bmatrix} \quad (7)$$

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. The matrix element of 4 X 4 Hamiltonian is given as follows,

$$P = \frac{\hbar^2}{2m_0}\gamma_1\left(k_x^2 + k_y^2 + k_z^2\right) \quad (8a)$$

$$Q = \frac{\hbar^2}{2m_0}\gamma_2\left(k_x^2 + k_y^2 - 2k_z^2\right) \quad (8b)$$

$$R = \frac{\hbar^2}{2m_0}\sqrt{3}\left[-\gamma_2\left(k_x^2 - k_y^2\right) + 2i\gamma_3 k_x k_y\right] \quad (8c)$$

$$S = \frac{\hbar^2}{2m_0}2\sqrt{3}\gamma_3\left(k_x - ik_y\right)k_z \quad (8d)$$

The variables γ_1, γ_2 and γ_3 are the Luttinger parameters [16-19] which are the functions of the lattice parameters and hence includes the strain effect in the self-consistent solution of the Schrödinger and Poisson equations. Further optical gain [17] of the quantum well laser diode is obtained using the gain coefficient given in equation (9) as follows,

$$\gamma = \frac{m^*\lambda^2}{4\pi^2\hbar a n^2\tau}\int_0^{DL}\frac{-T(f_v - f_c)}{1 + (\omega - \omega')^2 T^2} \quad (9)$$

where, m^* is the reduced mass of the electron, λ is the wavelength, '2a' is the well width, τ is the life time of the electron, the integral limit DL is the device length and other variables have their usual meanings. The Fermi Dirac functions for electrons and hole are f_c and f_v and given by the following expressions.

$$fc = \frac{1}{e^{(E - E_{Fc})/k_B T} + 1} \quad (10)$$

$$fv = \frac{1}{e^{(E - E_{Fv})/k_B T} + 1} \quad (11)$$

At this juncture k_B is the Boltzman constant, T is the temperature in Kelvin, E is the transition energy, E_{Fc} and E_{Fv} are the chemical potentials. The quasi-Fermi energies are the functions of the electron density of the individual well and barrier region. In the following section the results obtained through simulation has been discussed.

III. Results and Discussion

Figure 2 reveals the variation of the confinement factor with the variation of Aluminum mole fraction, temperature, wavelength and well width. It has been observed that with the increase in the Aluminum mole fraction and well width the confinement factor increases nonlinearly. The increase in the confinement factor is being attributed due to the step index enhancement with the increase in the mole fraction and increase in the overall dimension of the quantum structure. However, with the increase in a temperature and wavelength the confinement factor founds to be decreasing. The corresponding effective index of temperature variations has been observed to be 3.3235, 3.2989, and 3.2773. With the increase in temperature the electron starts tunneling and reduces the electron density in the quantum well which further reduces the recombination rate which effects near field and the field intensity spread is observed to be more in the cladding regions. Similarly, for the increase in the wavelength the effective index is found to be decreasing from 3.4983 to 3.155. While, the step index for the wavelength 350nm, 375 and 400nm is calculated to be 0.4336, 0.3167 and 0.2232 respectively.

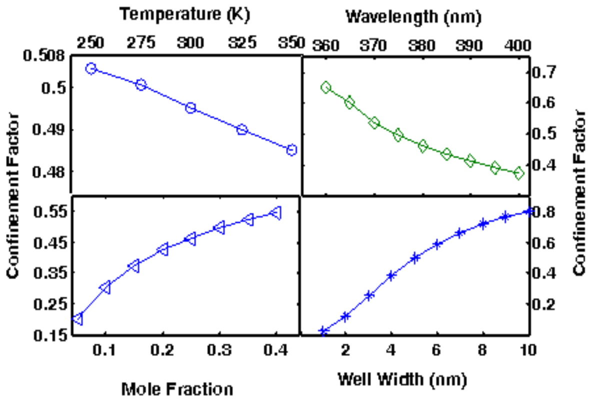

Figure 2 Dependence of confinement factor on various parameters.

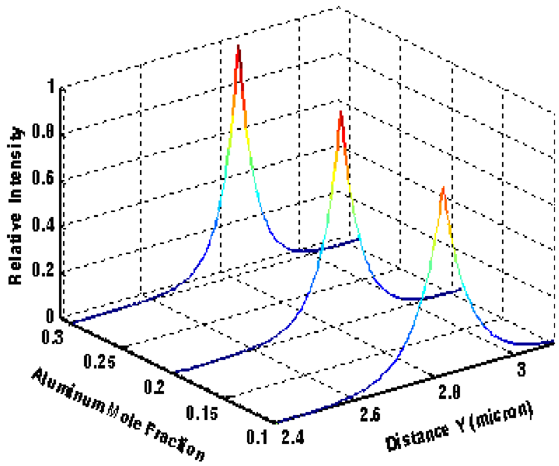

Figure 3(a) Near Field Intensity as a function of Aluminum mole fraction.

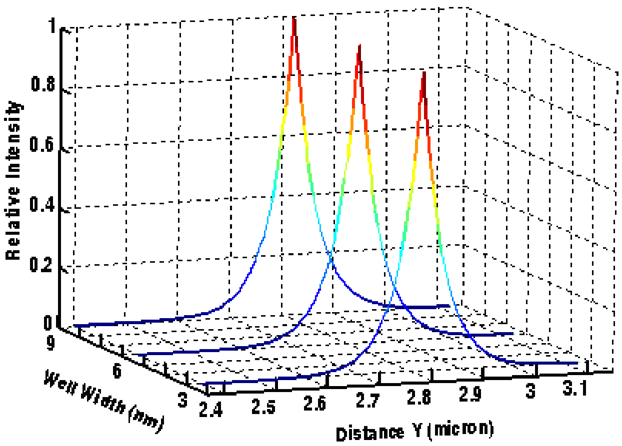

Figure 3(b) Near Field Intensity as a function of Well Width

The near field analysis has been carried out for the variation of Aluminum mole fraction and well width as shown in Fig. 3(a) and 3(b). The near field emerged to be dominant with the increase of both parameters viz. Aluminum mole fraction and well width. The increase in the mole fraction increases the step index and hence the effective index subsequently. With, the increase in the Aluminum concentration from 10% to 30% the step index increase from 0.1340 to 0.3167, while the refractive index variation of $Al_xGa_{1-x}N$ observed to be from 3.1651 to 2.9824. The effective index for the varying well width at room temperature and at 375 nm wavelength shows a minor variation 3.2986 to 3.2991. Since, the effective index increases the field intensity for greater well width has a dominant peak.

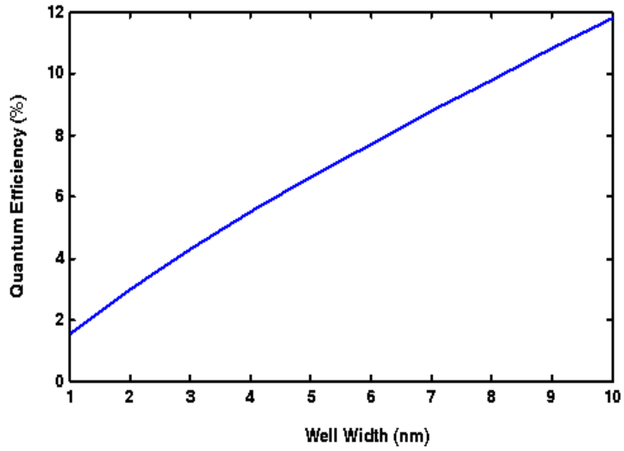

Figure 4(a) Quantum Efficiency variation with Well Width

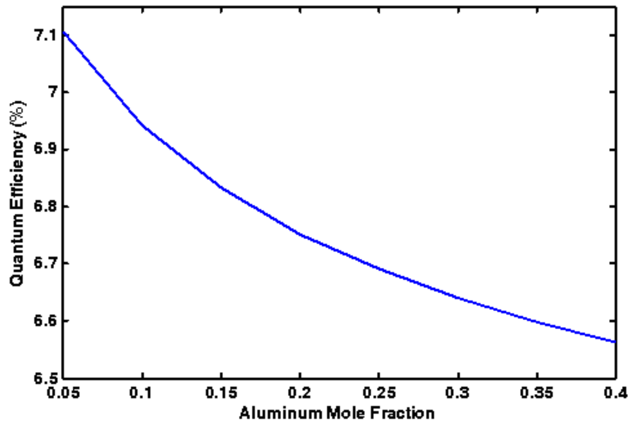

Figure 4(b) Quantum Efficiency variation with Aluminum Mole Fraction

Figure 4(a) and 4(b) shows quantum efficiency variation with well width and Aluminum mole fraction. During analysis we observed that the internal loss shows a nonlinear decrease with increases in the well width, while the quantum efficiency increases as shown in Fig. 4(a). The quantum efficiency is enhanced with the well width due to the localization of the carriers which amplifies the electron hole interaction [20].The lowering of the quantum efficiency with the increasing Aluminum concentration has been observed in our analysis as shown in Fig. 4(b). The increase in Aluminum mole fraction enhances the band offset between the well regions and thus restricts the carriers within the well region. Furthermore, the increase in Aluminum mole fraction in $Al_xGa_{1-x}N$ increases the step index between the well and the claddings which reduces the quantum efficiency. Here, the quantum well width was taken to be 5 nm while the wavelength used in calculation is 375 nm.

IV. Conclusion

The efforts have been made to optimize the physical and material properties to achieve reduction in carrier losses, along with minimization of self-heating to achieve higher quantum efficiency. We have achieved much better quantum efficiency of 12% for 0.3 mole of Aluminum in AlGaN. The results had revealed that a better optical confinement and higher quantum efficiency are achieved.

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His research thrust area is nano-simulation tools for quantum structure, computer simulation of semiconductor and optoelectronics devices, Materials development and characterization for the nano-technological and optoelectronics applications. He has developed with his research student a novel model of probability density spreading in GaN quantum wells and microcontroller based spin coating system for the deposition of nano-materials. He has guided many students for their innovative research.