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Field Intensity Distribution in Hetero-Structure Laser

S. A. Gaikwad

Associate Professor, Dept. of. Physics, ASC College, Varangaon, Bhusawal (M.S), India.

Email: israelgaik444@gmail.com

ABSTRACT

The computer aided simulation tools are of significant interest to access the device performance and to know in advance the device behavior before the actual fabrication and characterization process. We have carried out the numerical simulation of hetero-structure laser in the direction to develop an indigenous design tool which enables to better understand internal device physics and to optimize various structural, physical and material parameters which are required in the design of semiconductor laser. This simulation has been carried out using static device modeling approach for the analysis and optimization of various physical parameters. The wave equation is solved to get the optical field intensity distribution in various layers across the device is obtained. The modal analysis of optical confinement in three Layer hetero-structures are carried out to obtain the optimized set of structural parameters for maximum intensity. The basic electrical equations have also been implemented in discretized form and solved numerically to obtain the electrostatic potential and quasi Fermi potential at various nodes across the finite difference mesh of the device structure. The self-consistent solution of basic electrical and optical equations has been obtained by iterative solution procedure. The Simulation program is interactive and generates 3D surface profiles for optical intensity, electrostatic potential, quasi Fermi potential, carrier density distribution etc. at mesh nodes in the device. The other results are presented in graphical form for various combinations of material and structural parameters

Keywords: *Computer aided simulation tools, Field Intensity Distribution, Hetero-Structure Laser*

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Introduction

Nowadays, III–V compound semiconductors provide the materials basis for a number of well-established commercial technologies, as well as in short wavelength lasers. The operating characteristics of these devices depend on the physical properties of the constituent materials. Although, light sources using GaN [1] based compounds have been realized successfully, there is lot of scope remains to improve the efficiency of these devices by studying their physical mechanism on the basis of material properties to enhance their performance and characteristics. The GaN/AlGaN hetero-structure devices [2] are much more efficient for proper optical confinement at room temperature operation of the laser diode. To understand the internal physical mechanism of such diode, the analysis and optimization of its physical and material parameters [3] diode laser need to be carried out to evaluate actual device performance for its effective application. These parameters are closely related to optical and electrical behavior of the device and they give clear insight of high level effects which are very significant for device optimization. Section II, of the paper describes the static device modeling of self-consistent electrical and optical equations and methodology to implement and solve these equations in the device structure. Section III, describes the simulation results obtained from theoretical models for various components under different operating conditions and parameters.

II. Laser Diode Modeling:

(A) Optical Equations:

One of the most important optical equations to describe the performance of optical devices is the wave equation. By applying proper hetero-interface conditions we have optimized field solutions in different layers of the hetero-structure device. Eigenvalue equations were used to obtain the effective refractive index, N. Propagation constants in different layers of the device were computed using the following formulas:

$\gamma_c = \sqrt{\kappa_0 [N \; - n_c]}$ in the clad,

$\kappa_x = \sqrt{\kappa_0 [n_f - N \;]}$ in the active layer.

$$V \times \sqrt{1 - b_E} = m - \tan^{-1}\sqrt{(1 - b_E)/(b_E + a_E)}$$

where γ_c is the propagation constant in clad, k_0 the free space propagation constant for wavelength under consideration, k_x the propagation constant in active region, n_C the refractive index of clad region, n_f the guiding layer refractive index, V the normalized frequency, b_E the normalized guide index, a_E the asymmetry measure of wave guide, being zero for our symmetric hetero-structure, m=0, 1…is the mode value.

Field solutions have been obtained from the wave equation by using normalization conditions and hetero-interface conditions along the Y-direction of the device as:

$$E_y = E_{uc} * \exp(-\gamma_c y)$$ in upper clad,

$$E_y = E_f * \cos(k_x * y + \phi_c)$$ in active layer,

$$E_y = E_{lc} * \exp\{\gamma_c (y + d)\}$$ in lower clad, with

$$\phi_c = \tan^{-1}\left(\frac{\gamma_c}{k_x}\right)$$

where E_y represent field intensity, E_{uc}, E_f, E_{lc} are the coefficients in general solution of wave equation in upper clad, active layer and lower clad respectively, ϕ_c the phase angle, d the active layer thickness. The field equations are solved to analyze the laser diode structure shown in Figure 1. Thus, the above solutions are helpful to reveal the relative intensity in different layers. The structural parameters used for the analysis are listed in Table 1. For the different thicknesses of the various layers, the corresponding relative intensities are observed.

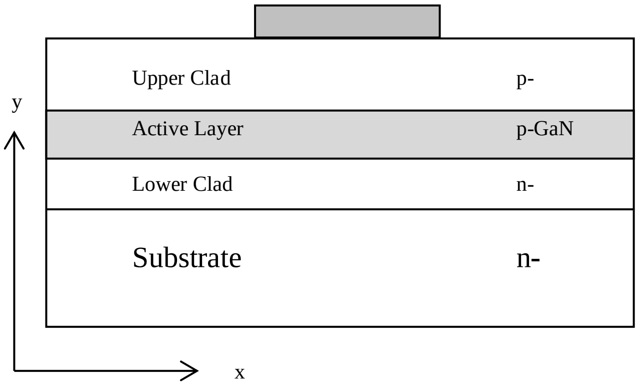

Figure 1: Typical Structure of Laser diode.

Layer	Thickness (µm)	% of Al	Refractive Index
Substrate	3.00	00	2.6907
Lower Clad	0.38	10	2.5830
Active Region	0.30	00	2.6907
Upper Clad	0.40	10	2.5830

Table 1: Structural parameters used for the analysis.

(B) Electrical Equations:

Poisson's Equation and continuity equations for electrons and holes describe the electrical behavior of semiconductor hetero-structure laser diodes. Poisson's equation is used for analyzing the potential distribution in the device. The Poisson's equation for a double hetero-structure in which dielectric constant, (having a spatial dependence is expressed as,

$$\nabla.(\varepsilon\nabla\psi) = -q\,(p - n + N_d - N_a)$$

Where ψ is the electrostatic potential , q is the electronic charge, n is the electron density and p is hole density, N_d is concentration of donors and N_a is a concentration of acceptors in various layers of hetero-structure. We apply the boundary conditions to determine the electrostatic potential and quasi Fermi potential at free boundaries of the given structure. The following equations give the free boundary conditions,

$$\nabla\psi\,|_{normal} = 0, \nabla\phi_n\,|_{normal} = 0 \text{ and } \nabla\phi_p\,|_{normal} = 0$$

The quasi Fermi potentials at the contact are given by $\phi_n=\phi_p=V$ where, V is an external bias. Electrostatic potential at contact is obtained by fixed boundary condition as,

$$\psi = V_t \times \sinh^{-1}\left[\frac{N_d - N_a}{2n_i}\cdot\exp\left(\frac{\gamma_n-\gamma_p}{2V_t}\right)\right] + \frac{\gamma_n-\gamma_p}{2} + V - \theta$$

Where, γ_n and γ_p are degeneracy parameters for electrons and holes respectively, n_i is intrinsic concentration, V_t is thermal voltage and V is an external applied bias and θ is the band parameter which describe the discontinuities of the electron affinity and the band gap.

Carrier densities are having spatial and time dependence in continuity equations for static and dynamic analysis of semiconductor devices. The time dependence of these equations is not considered in static modeling. The total charge transport in semiconductors is constituted from electron and hole transportation in the conduction and valence band respectively. Therefore, continuity equation needs to be considered for each type of carriers. These equations are used to obtain quasi-Fermi potentials for the electrons and holes throughout the device structure. The electron and hole densities are related with electron current density and hole current density respectively by the electron and hole continuity equations as follows,

$$\frac{\partial n}{\partial t} = -\frac{q1}{q}\nabla \cdot \ddot{J}_p + G - R$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q}\nabla \cdot J_p + G - R$$

Where, J_n is current density for electrons, J_p is the current density of holes, G is carrier generation rate and R is the carrier recombination rate. For static modeling of the device, time dependence of these equations is not considered but only the space dependence of these equations need to be considered. In these equations, J_n and J_p are further given as:

$$J_n = -q\mu_n n\nabla\phi_n \qquad J_p = -q\mu_p p\nabla\phi_p$$

Where, μ_n is mobility of electrons, μ_p is mobility of holes, ϕ_n is quasi-Fermi potential for electrons and ϕ_p is quasi-Fermi potential for holes. Values of J_n and J_p are substituted into the continuity equations to obtain simplified expressions for solving quasi-Fermi potentials for electrons and holes. By solving Poisson's equation and continuity equations for electrons and holes, we have obtained values of electrostatic potentials and quasi-Fermi potentials for electrons and holes at various points in the device structure. After knowing all these values, the electron and hole densities at various points in the device structure are obtained using following equations:

$$n = n_i \exp\left[\frac{(\psi + \theta - \gamma_n) - \phi_n}{V_t}\right]$$

$$p = n_i \exp\left[\frac{\phi_p - (\psi + \theta - \gamma_p)}{V_t}\right]$$

Where, $V_t = \left(\frac{K_b \cdot T}{q}\right)$ is the thermal voltage. The band parameter θ is the energy difference between vacuum level and the intrinsic Fermi level and expressed as,

$$\theta = -V_{ref} + \chi + \frac{E_g}{2} - \frac{V_t}{2} \times \log_e \frac{N_v}{N_c}$$

Where, V_{ref} is the reference potential, χ is electron affinity, E_g is energy band gap, N_v is effective densities of states in the valence band, N_c is effective densities of states in the conduction band. The degeneracy parameters γ_n and γ_p are given by,

$$\gamma_n = V_t \times \log_e \left(\frac{\exp(Z_n)}{F_{1/2}(Z_n)} \right)$$

$$\gamma_p = V_t \times \log_e \left(\frac{\exp(Z_p)}{F_{1/2}(Z_p)} \right)$$

Where,

$$Z_n = \frac{E_c - \phi_n}{V_t} \quad \text{and} \quad Z_p = \frac{\phi_p - E_v}{V_t}$$

Where, E_c and E_v are the conduction and valence band energies respectively. $F_{1/2}(Z_n)$ and $F_{1/2}(Z_p)$ are the Fermi-dirac half integrals of Z_n and Z_p respectively.

(C) Methodology:

GaN/AlGaN laser performance is predicted on the basis of numerical solutions for basic device equations under steady state. The simulation program has been developed for the planer diode laser structure shown in Fig. 1. For this purpose the device structure has been transformed into a mesh having several nodes. We have applied finite difference method for two dimensional mesh structures for solving the basic electrical equations in the device. The structural parameters of diode laser, composition and doping concentration of various layers are given as inputs to the program and material constants are evaluated. The numerical values of physical parameters of GaN and its ternary alloys like AlGaN are obtained from experimental and theoretical data available. The change of material parameters from layer to layer has been considered while solving the equations.

Simulator assigns the initial values of quasi Fermi potential to all nodes at fixed and free boundaries of rectangular structure and evaluates the quasi Fermi potential at remaining internal node points using the standard difference formula. Array of quasi Fermi potential is further used for numerical estimation of the electrostatic potential at various nodes in mesh structure. The simulator executes the program for Poisson’s equation and continuity equations, number of times iteratively in self-consistent manner till the equation is converged to sufficient accuracy. The results of solution of optical equations are coupled to the computational results of electrical equations through stimulating the recombination rate which is used in the continuity equation.

III. **Results:**

Mode Confinement:

Figure 10 shows the Intensity distribution across the device for mode 0 and 1 computed for the light of wavelength 375nm. For mode 0, the relative Intensity is seen exponentially increasing in lower clad & exponentially decreasing in upper clad and reaching to maximum inactive region. Mode 0 is seen more confined as compared to mode 1, therefore cavity supports mode 0 as it exhibits higher intensity for it. It is clear from Figure that the mode 0 shows strong optical confinement within the active layer. However, mode 1 did not show excellent confinement within the active layer due to its very smaller thickness. Also, it exhibited more losses as compared to mode 0.

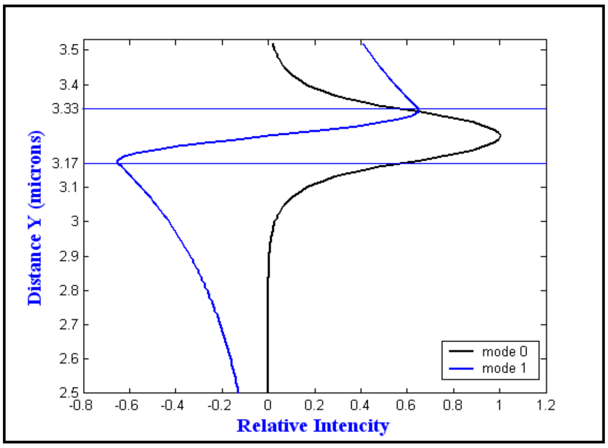

Figure 10: Intensity distribution across the device for mode 0 and 1.

Field Intensity Distribution:

Figure 11 shows confinement of near field intensity across the layers of device for different values of the Al mole fraction which is plotted against Y distance in microns. Increase in field confinement with mole fraction has been attributed to increase of refractive index step between the active layer and cladding layers as we increase Al contents in cladding material.

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The increase of refractive index step of hetero-structure enhances the magnitude of the effective refractive index. The full width at half maximum (FWHM) of near field intensity was computed and it was estimated to be 0.25 and 0.21 microns corresponding to Aluminum mole fractions of 5% and 15% respectively. Increasing the mole fraction increases the intensity and confinement also, this is due to increase in band gap discontinuity of hetero-structure. Our analysis reveals that with increase in Al mole fraction the optical confinement increases significantly.

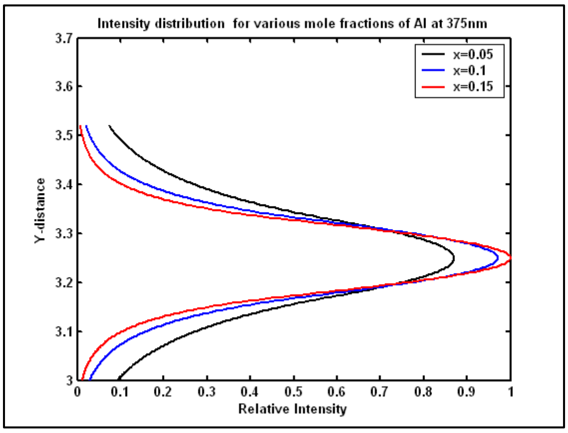

Figure 11: Effect of variation in mole fraction of Al in clad on relative intensity.

Effective Index Dependence On Mole Fraction, X:

Figure 12, shows the variation in the effective index of the structure with the Al mole fraction. The refractive index of $Al_xGa_{1-x}N$ decreases with increasing Al mole fraction, therefore the effective index of the structure decreases with increase in mole fraction. The optimization of the effective index at a given wavelength is very significant as it directly affects the device performance and also determines the degree of electrical and optical confinement of the diode laser. The effective index is found changing nonlinearly with mole fraction of the light of 375nm wavelength. The rate of change of effective index is more for lower molar compositions and it slows down for molar concentrations higher than 50%.

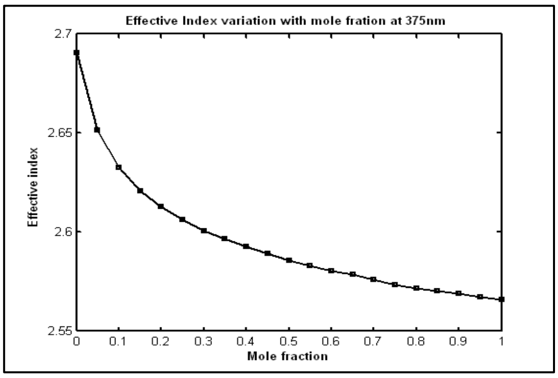

Fig.12: Effect of Al mole fraction on effective index of the planar structure.

(a) Quantum Efficiency:

We have studied the effect of cavity length of laser diode on its quantum efficiency. Figure 13 shows the dependence of quantum efficiency on the cavity length. It was observed that the quantum efficiency decreases nonlinearly with an increase of cavity length, due to increase in the cavity losses. Our analysis reveals that the differential quantum efficiency is 12.5% for the cavity length of 300µm. The stimulated efficiency was assumed to be 0.35 and internal losses in the cavity includes absorption loss, mirror loss and free carrier loss. For a fixed bias of 6 V, free carrier loss was found to be 30 cm^{-1}. Assuming thicker cladding layers in hetero-structure lasers, absorption loss in the substrate is assumed very low and its value is taken as 10 cm^{-1}.

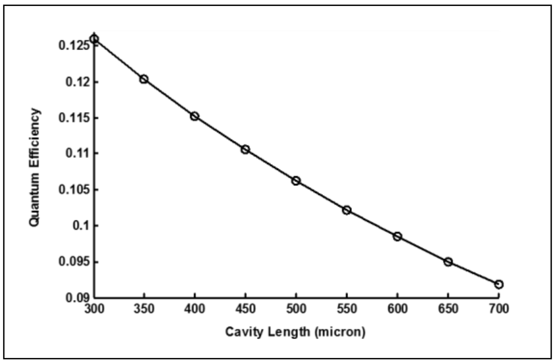

Figure 13: Effect of cavity length on the quantum efficiency of laser diode.

IV. Conclusion

The computer aided simulation tools have been developed for the analysis and optimization of structural and material parameters of GaN/AlGaN hetero-structure laser. The self-consistent solution of basic electrical and optical equations has been obtained by iterative solution procedure. The results are optimized for the lasing wavelength of 375nm. Analysis of mode confinement, field intensity distribution for various mole fractions of Al, effective index dependence on the Al mole fraction and dependence of quantum efficiency on cavity length has been carried out to explore applicability of nitride lasers operating at room temperature. The output results obtained from our analysis demonstrate clearly the usefulness of this work in the design of nitride based semiconductor laser.

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