SIMULATOR FOR SOLVING POISSON'S EQUATION IN GAN/ALGAN DOUBLE HETERO-STRUCTURE LASER DIODE

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Abstract: GaN/AlGaN materials are very important to fabricate low wavelength lasers. It is desirable to develop the simulator to study these devices. Numerical simulations have been carried out to solve the Poisson's Equation in two dimensions in the given structure to obtain the potential distribution in the device. The structural parameters used in simulation are length (700µm), width (50µm) and thickness (3.520µm). A simulator has been developed which receives the structural and material parameters and estimates the electrostatic potential at each node point in various layers in the device. For this purpose, the device structure has been transformed in to a mesh having 65x50 node points. The boundary conditions are applied and potential at fixed and free boundary is estimated. The potential at fixed boundaries are calculated by considering the donor and acceptor concentrations and band degeneracy parameters. By applying the forward difference formula the potential at each node point has been estimated. The Poisson equation is solved to get potential at each node point in device. The simulator generates the 3D surface profiles of the potential distribution in the hetero-structure laser diode. The numerical values of potential at various points are required in design and analysis of semiconductor laser diodes. We have carried out efficient computational analysis using MATLAB tools so as to reduce number of iterations. This paper will high light the details of methodology and results with their analysis.

***IndexTerms* - Laser diode, Hetero-structure, Band degeneracy, Simulator, MATLAB.**

I. INTRODUCTION

Gallium nitride is a semi conducting compound material of high technological importance with a variety of applications in optoelectronics, high-power and high-temperature devices. It is used in number of optoelectronic and electronic materials including Laser diodes[1], LEDs[2], Photo detectors [3] etc. The nitride based diodes have several applications in variety of fields including optical communication systems, display devices, optical storage devices and optical data processing systems. The compounds of GaN have active potential for light emission in visible to ultra-violate range of frequencies. In this work an attempt has been made to conduct the numerical simulation of GaN/AlGaN laser diode with the experimental data available for nitride based laser diodes. The recent developments in fabrication technology has made it possible to grow good quality of AlGaN layers with controlled band gap and lattice matching with GaN substrate. The AlGaN serves as an optimum material for carrier stopper layer along with GaN as an active layer which is having the band gap of 3.42 eV [4] . In order to fabricate improved laser diode for a particular application it is very important to optimize its fundamental physical and material parameters.

In this paper we present the numerical analysis of GaN/AlGaN double hetero-structure carried out to solve the electrical equations. Section II describes Laser diode modeling used for analysis and the device structure along with corresponding dimensions under consideration are depicted in Section III. The methodology used for numerical simulation of Poisson's equation is described in section IV. Results and observations are discussed in section V followed by conclusions and acknowledgement.

2. LASER DIODE MODELING:

Laser diode is an optoelectronic device which involves complex process of light generation and amplification when properly biased to provide enough current more than threshold value. For constructing efficient light emitting devices one should select the perfect material having band gap corresponding to desired wavelength and optimize the entire structure. For doing this the numerical values of physical parameters of the material are required to be considered. We have used the recent experimental data [5,6] to obtain the material parameters such as carrier mobility, carrier effective mass, doping concentration, band gaps etc.

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, ε having a spatial dependence is expressed as

$$\nabla . (\varepsilon \nabla \psi) = - q\,(p - n + N_d + N_a) \qquad (1)$$

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

$$\nabla \psi \,|_{normal} = 0, \nabla \phi_n \,|_{normal} = 0 \text{ and } \nabla \phi_p \,|_{normal} = 0 \qquad (2)$$

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

$$\psi = V + \{V_t * \sinh^{-1} [(0.5(N_d - N_a)/n_i) * \exp(0.5(\gamma_n - \gamma_p)/V_t)] - \theta + 0.5(\gamma_n - \gamma_p)\} \qquad (3)$$

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.

The band parameter having dependence on the composition of material is introduced to describe the discontinuities of the electron affinity and the band gap. The band parameter[7] which gives the energy difference between vacuum level and intrinsic Fermi level is modeled separately and it has been calculated by considering reference voltage, band gap and electron affinity for each layer in the structure. The band degeneracy has been calculated for electrons by considering conduction band energy and quasi Fermi potentials for the electrons and the degeneracy for holes include valence band energy level and quasi Fermi potential for the holes. The Fermi half integrals[7] for electrons and holes have been calculated using analytical approximations.

3. DEVICE STRUCTURE:

The GaN/AlGaN semiconductor planer laser diode structure consisting of substrate, lower clad, active region and upper clad is used for simulation as shown in Fig. 1. The structure contains GaN substrate with thickness of 3 μm on which $Al_{0.3}Ga_{0.7}N$ carrier stopper layer adjacent to active layer is used in both the conduction and valence bands to confine the carriers to active layer. The GaN center region is the active region where most of the light is generated and amplified in the cavity. The energy gap of active region is lower than that of energy gap of cladding layers to have confinement of carrier for the radiative recombination. The energy gap strongly depends upon Al mole fraction in the clad and active region. The refractive indices in substrate, clad layers and in active region are dependent on doping concentration and Al mole fraction. The refractive index of active region is greater than that of cladding layers to have proper optical confinement. The various layers along with their doping concentrations and thicknesses considered in the simulation are also shown in the Fig. 1. The structural parameters of the device used in simulation are length (700μm), width (50μm) and thickness (3.520μm). By using these structural parameters Poisson’s equation is solved, iteratively in a self-consistent manner until the solutions get converged with sufficient accuracy.

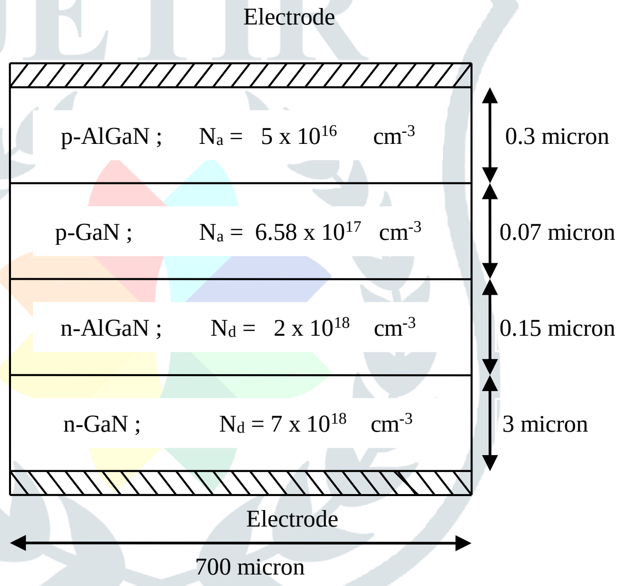

Fig 1: Structure of the simulated device with doping concentration and alloy composition fractions.

4. METHODOLOGY:

Hetero-structure device performance is predicted on the basis of numerical solutions for basic device equations under steady state. The simulator has been developed for planer diode laser structure Fig. 1. For this purpose the device structure has been transformed in to 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[5]. The change of material parameters from layer to layer have 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 standard difference formula. Array of quasi Fermi potential is further used for numerical estimation of electrostatic potential at various nodes in mesh structure. The simulator executes the program for Poisson’s equation number of times iteratively in self-consistent manner till the equation is converged to sufficient accuracy of the order of 10^{-7}. By solving Poisson’s equation we have obtained values of electrostatic potentials and quasi Fermi potentials for electrons and holes at various points in the interior of the device.

5. RESULTS AND DISCUSSION:

In this section we present the results of our simulation demonstrating the device performance under various biasing conditions. The device simulator has been developed in MATLAB, which solves Poisson's Equation at each node point in the device and estimates electrostatic potential distribution in the device at several mesh points whose numerical values are stored in an array. Fig. 2 shows the potential distribution within device for an external bias of 3 Volts. It reveals that electrostatic potential is almost constant in horizontal direction at different nodes along the rows (i.e. length) and it is changing at nodes along the columns (i.e. thickness) layer to layer. Potential distribution is uniform in substrate due to its higher thickness of 3 microns. In the design and analysis of diode laser it is required to converge the Poisson and continuity equation for carriers in a self-consistent manner. The simulator estimates the potential at each node point, which is required in solving continuity equation which in turn determines the carrier concentrations.

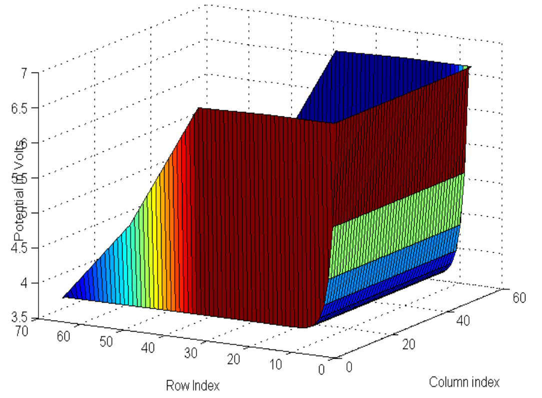

Fig. 2. Potential Distribution in the device represented by corresponding row and column node points in mesh structure.

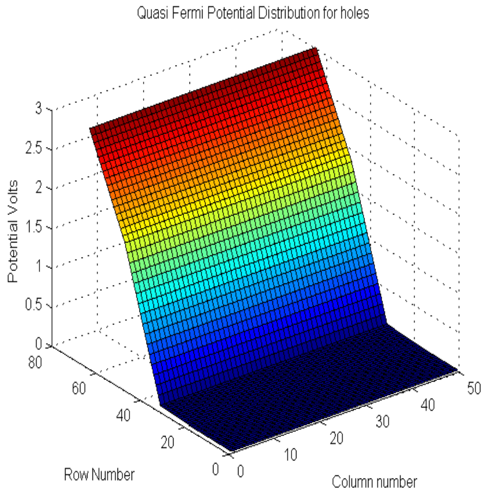

Fig. 3. Quasi Fermi Potential Distribution for holes.

It is also observed that there is a reduction in potential at the interface of the boundary of layer this is due to step in dielectric constant of hetero-structure which is formed of various layers. Fig. 3 is the potential distribution profiles for quasi Fermi potential for holes. The quasi Fermi potential is almost constant in horizontal direction at different nodes along the rows (i.e. length) and it is changing at nodes along the columns (i.e. thickness) layer to layer. The quasi Fermi potential is almost zero in substrate and lower clad and it then increases uniformly and having maximum value at the boundary of upper cladding layer.

6. CONCLUSION:

We have performed a numerical simulation of a wide band gap GaN/AlGaN hetero-structure diode laser which include the stopper layer around the active region for greater carrier confinement. Fast and convergent algorithms are designed for solving Poisson's equation in device using MATLAB 7.14. The execution time to converge Poisson's equation depends upon the choice of initial input values and accuracy needed. For complete simulation of semiconductor laser and its optimization the Poisson's equation and continuity equation in a self-consistent manner along with photon density equation needed to be solved. The solution of Poisson equation gives the numerical values of electrostatic potential at each point with the device and on its boundaries. These potentials are required in solving continuity equation in the device which is required in design, development and analysis of semiconductor laser diode.

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