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Analysis of electron confinement in quantum well biased laser diode using quasi transmitting boundary method

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We have solved Schrödinger wave equation to study the quantization and electron transport behavior in finite quantum well of GaN/AlGaN biased laser diode. The study of electron confinement in single quantum well has been carried out by using quasi transmitting boundary method for complete numerical solution of the quasi bound states. The wave functions have been deduced using finite well potential energy for the varying applied bias voltage. Computer simulation tools have been developed using MATLAB to study distribution of wave function within the quantum well biased laser diode. The spread of the probability density has been obtained by estimating the full width at half maximum (FWHM) with the quantum well thickness of 5 nanometer, 30% Aluminum mole fraction for different values of bias voltage. The probability density shows greater spread for the lower value of bias voltage. It further reveals that electron energy increases nonlinearly with the increase in electric field.

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1. Introduction

III-V nitride semiconductors such as GaN have long been considered to be pertinent materials in light emitting device applications. The band gap of the nitrides ranges from 1.8 eV of InN, 3.39 eV of GaN to 6.3 eV of AlN, are eventual candidates for light emitting diodes and laser diodes in the ultraviolet-green wavelength regimes. Hence, the direct nature of its band gap makes GaN ideal for optical detection and emission within the ultraviolet portion of the electromagnetic spectrum. The Short wavelength lasers using these compounds have been realized as efficient light sources. Semiconductor light sources operating in the UV region are required for a number of applications, including long lifetime white lighting, sterilization, decontamination, , in biochemical processes, for the purification of the environment, and for high-density optical storage [1-5].

There has been a growing interest in the optical and electrical properties of nitride films due to several recent advances. Energy band offsets dominantly control the electronic states in heterostructures and, hence, the output parameters of light emitting devices. The physics of tunneling phenomena in semiconductor quantum well laser diode has been a subject of considerable investigation since the early work of Tsu and Esaki [6]. A number of theoretical works have been developed for understanding and simulating the behavior of carrier tunneling in quantum well structures [7]. The physics of semiconductor nano-devices, in particular double heterostructure quantum well (QW) lasers, is influenced significantly by the interaction of electrons and holes with the lattice vibrations of the heterostructure. Different experimental [8-10] and theoretical methods have been devoted to investigate the electronic structure of the interacting electrons confined in quantum well under the effect of an applied electric field. One of the most interesting features of electrons confined in quantum well is the energy level crossing.

The device application of the quantum wells in a resonant tunneling structure has also been demonstrated [11]. We consider a quantum well with an electric field. The electron confinement in a quantum well with an applied electric field is investigated here. The wave functions of the electrons and holes are those of the displaced harmonic oscillators, which are shifted in opposite directions. The analytical expressions here illustrate for the electron wave function in quantum well structure. The Schrödinger equation has been solved by using quasi transmitting boundary method (QTBM) developed by Lent and Kirkner in 1990 [12]. The paper presents the theoretical clarification in section 2; section 3 includes the results and discussion, while the conclusion is provided in the final section 4.

2. Physical model

Electron exhibits interference and diffraction phenomena. Therefore, the electron can behave as a wave under certain conditions. The carrier charge density is determined by the solution of Schrödinger equation for the wave function of the carriers in the layered quantum system. The solutions known as general solutions of Schrödinger equation describe the wave like behavior, with the appropriate potential energy and boundary conditions. The Schrödinger equation including the electric field is expressed as follows.

$$-\hbar^2/2m^*d^2\Psi(x)/dx^2+(V+eFx)\Psi(x)=E\Psi(x) \qquad (1)$$

where m, is the mass of the electron
e, is the electron charge
E, is the energy of the electron
F, is the electric field

The potential energy V is the superposition of the potential energy due to conduction band offset at the interfaces between the layers, which are arises from the presence of ionized donors and the free charges released by them. For bound states, the wave function is zero at the left and right boundaries, far into the barrier regions. These boundary conditions are now built into the set of simultaneous equations are given below.

$$\Psi_1(x)=Ce^{\kappa x} \qquad (2)$$

$$\Psi_2(x)=A\cos kx+B\sin kx \qquad (3)$$

$$\Psi_3(x)=De^{-\kappa x} \qquad (4)$$

where A, B, C and D are arbitrary constants.

At this juncture, $k=(2mE/\hbar)^{1/2}$,

$\kappa=(2m(V+eFx-E)/\hbar)^{½}$, $\hbar=h/2\Pi$

h is Planck's constant.

We have used quasi transmitting boundary method for the solution of Schrödinger equation for quasi bound states. We are concerned with the incoming and outgoing waves from well under a biased condition. This lead-in a modal analysis of the wave function in terms of incoming and outgoing component wave function at the two ends. While, using the quasi transmitting boundary method the probability density interpretation of the wave function must tend towards zero into the outer barriers. Hence, the structure as shown in Fig. 1 taken for developing the physics of two dimensional systems is more relevant with the alternating layers of dissimilar semiconductors and finite depth of the quantum well model.

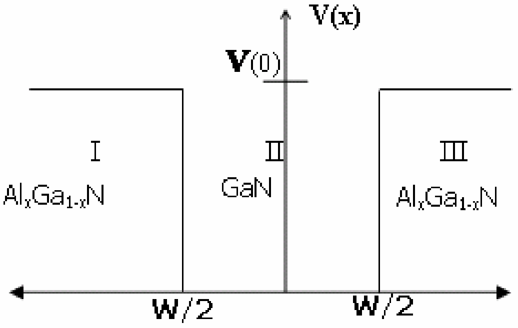

Fig. 1. GaN based Finite Quantum well Structure.

The general solutions of the Schrodinger equation for finite quantum well consisting of three regions are given below.

When we apply the boundary condition to the equation 2 to 4

The transcendental equations obtained are,

$$k^*\tan ka=\kappa \qquad (5)$$

$$\kappa^*\tan ka=-k \qquad (6)$$

The transcendental equation 5 and 6 are solved either by graphically or by numerical methods. As both k and κ are the function of electron energy E, the transcendental equations were solved by iterative numerical approach to determine the electron energy E first from which the both wave vectors of barrier and well region κ and k respectively were calculated.

3. Results and discussion

The quasi transmitting boundary method has been used to obtain the transcendental equations to observe spreading of wave function in the quantum well structure. Fig. 2 shows the three dimensional wave function distributions in X-Y plane of the quantum well laser diode structure without considering the biasing. It was found from our analysis that the wave function shows its peak amplitude in the quantum well region and less spread for the 30% aluminum mole fraction in the barrier region. The peak amplitude obtained in the quantum well region is due to the band offset at interface of well and barrier region. This electrical phenomenon of the quantum well structure enhances the electrical and optical gain of the laser diode.

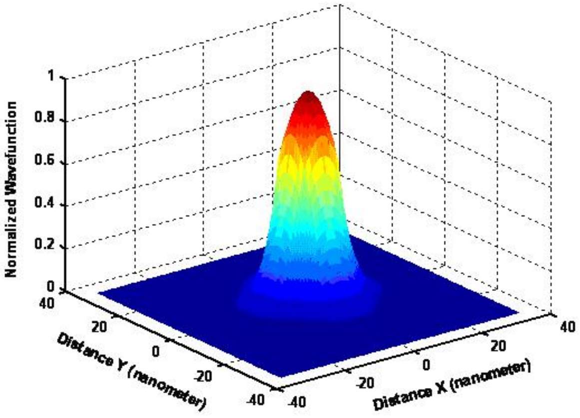

Fig. 2. wave function distributions in X-Y plane without biasing.

For, the simplicity the quantum well structure was taken to be symmetrical along X and Y axis. Therefore, in Fig. 3 we observe a bright spot exactly at the centre, which indicates a better electron confinement in the quantum well in X-Y plane. The electron confinement is necessary to cause the recombination and further stimulated emission of photons. Darker region on the remaining side indicates the tunneling of electron up to some extent.

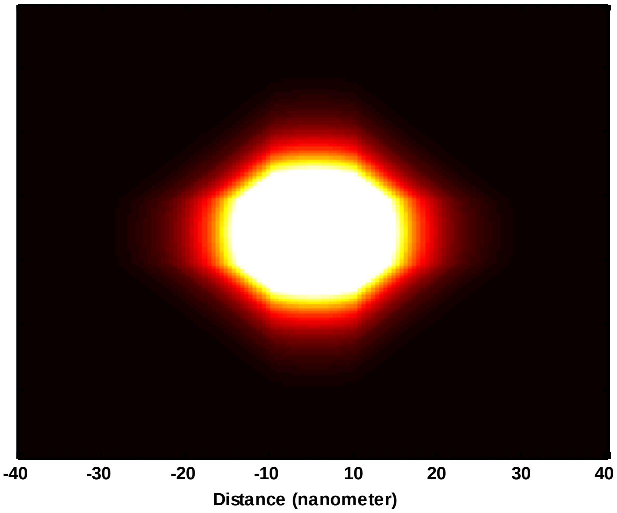

Fig. 3. Surface image of wave function distribution in X-Y plane without biasing.

The electron velocity GaAs, GaN, InP and most other III-V compound semiconductors, decreases with an increase in the electric field F. When the electric field is low, electrons are primarily located in the central valley of the conduction band. Hence, with the increase in the applied bias voltage the peak amplitude of the electron wave function distribution decreases as it is reveled in Fig. 4. It is due to the fact that the electron at higher electric fields shifts to satellite valley from central valley. In satellite valley the effective mass of the electron is increased and hence the differential mobility becomes negative which drastically effects to the electron transport phenomena. The electron distribution function has been realized for varying applied bias voltage from 3V to 5V. The Fig. 5 divulges the image of the electron confinement in the quantum well region. The image figure corresponding to 3V has a higher intense region as compared to those of 4V and 5V. Thus, it is concluded from the figure optimization is highly necessary to obtain a better optical and electrical gain of quantum well laser diode.

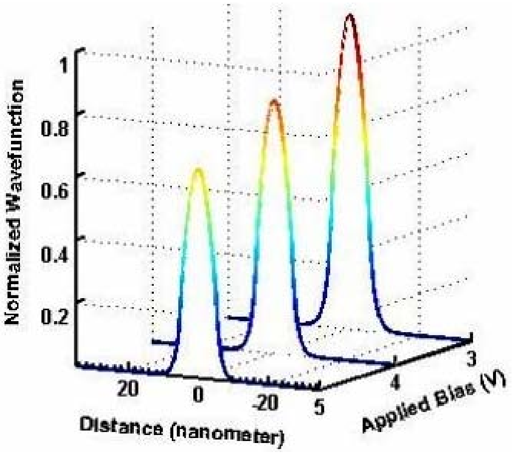

Fig. 4. Wave function distribution in along X-axis with applied electric field.

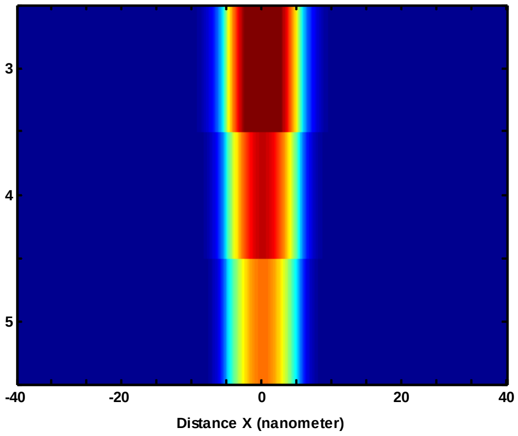

Fig. 5. Surface image of wave function distribution in along X-axis with applied electric field.

The width of the quantum well is considered to be 5 nanometer, while the total device length is taken to be 80 nanometer. The electrical field effects on the electronic and optical properties of quantum well structure based laser diode. Hence, the spread of the electron wave function distribution has been analyzed as shown in Fig. 6. The full width at half maximum (FWHM) of the electron distribution function shows a non-linear decrease with the increase in applied voltage. The FWHM of the wave function under unbiased condition was observed to be 14 nanometer, while the spread decreases to 9.4 nanometer with the increase in biasing (5V). In Fig. 7 the electron energy has been shown as function of the electric field. The electron energy founds to be increase non-linearly from 357 meV to 598 meV with the increase in an applied voltage. The electron energy is obtained by using the quasi transmitting boundary method and applying the numerical iterative method to the transcendental equations of the wave vectors. Since, the wave vectors are the function of electron energy hence the wave function of the electron is greatly depends on the electron energy. The increase in the electron energy causes the electron gain enough energy to get transfer from central valley to satellite valley. As, the electron energy gains the energy the effective mass in of the electron in the satellite valley is enhanced.

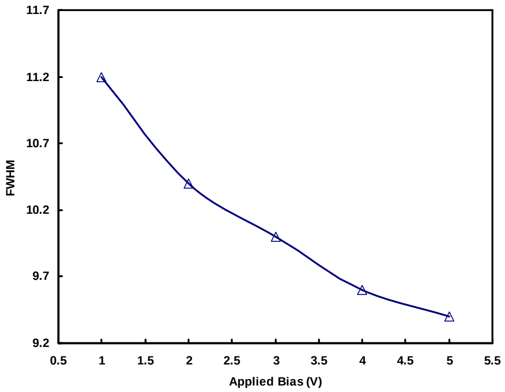

Fig. 6. FWHM of electron wave function distribution.

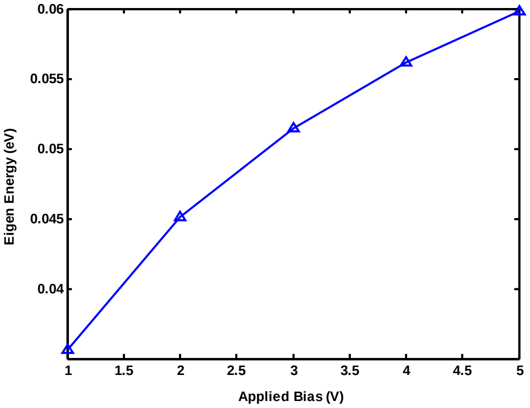

Fig. 7. Electron energy as function of applied voltage.

4. Conclusion

In this paper, we studied the electron distribution function under the bias conditions using the quasi transmitting boundary method. It has been observed that by increase in the electric field the decrease in the peak amplitude of the electron distribution function occurrs. This is due to the enhancement of the effective mass of the electron, decrease in the electron velocity and shifting of the electrons from central valley to satellite valley. The spread of the electron decreases with the increase in applied voltage.

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