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ANALYSIS OF WAVEFUNCTION DISTRIBUTION IN QUANTUM WELL BIASED LASER DIODE USING TRANSFER MATRIX METHOD

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Abstract—The paper presents the faster, simpler, and accurate algorithm to solve time independent Schrödinger equation based on transfer matrix method. We can thus calculate all bound and quasi bound energy and the corresponding probability density. A central part of this paper deals with the solving of Schrödinger equation for quantum well structure. Our results show that the transfer matrix method is accurate, it is easier to implement. The increase in well width increases the FWHM from 5.4 nanometer to 9.4 nanometer, while the increase in the Aluminum concentration the FWHM decreases from 8.98 to 5.4.

1. INTRODUCTION

In recent years semiconductor quantum wells have attracted growing interest for laser applications mainly due to their potential for a reduction of the threshold current density, and their increased gain and differential gain achieved by confinement. Since, quantum confinement of carriers in semiconductor quantum wells [1–7] leads to quantized subband energies. Parallel to the effort concerning the fabrication and characterization of quantum wells, their theoretical modeling are developed with increasing level of sophistication, in order to enable the prediction of the physical properties of such structures and to enable a deeper understanding of experimental results.

In semiconductor quantum structure, the rapid changes in the number of carriers leads to a electron transport phenomena due to which stimulated emission and electromagnetic radiations are occurred. The transferred electron effect in compound semiconductors occurs due to intervalley scattering are important in the operation of light

emitting devices. The III-V nitride semiconductors GaN, AlN, and their ternary alloys are highly attractive due to their great potential for development of shorter wavelength optoelectronic devices. Even though, remarkable progress in growth of GaN and their alloys and in fabrication technology of the devices using these materials, some basic properties of GaN/AlGaN still remain poorly studied [8–13].

In this paper we present a simple, accurate, and fast algorithm for numerically solving the Schrödinger equation for quantum well structure as shown in Figure 1. The wavefunction and Eigen energy profile under an applied electric field is as shown in Figure 2. The Eigen energy and wavefunction are obtained by the algorithm based on the transfer matrix method (TMM) [14–18]. The TMM is a general numerical method that can be used for a wide range of problems dealing with second order differential equations. One example is the calculation of propagation characteristics in planar wave guide, presented by Walpita [19]. One other example of the transfer matrix method is given in [20, 21], where the spontaneous emission in a DFB laser is investigated. The TMM is simple to implement and gives accurate results to three or four digits which is more than sufficient for most applications and this method gives quick and accurate answers to complex problems.

This paper is outline as follows, in Section 2, we will give a brief explanation of the theory behind the transfer matrix method and its implementation. Section 3 contains several examples of results obtained with our program carried out for single quantum well structure in an applied electric field and takes the variation of well width and the effective mass with varying Aluminum mole fraction in $Al_xGa_{1-x}N$. Finally, in Section 4 we present the conclusions.

2. SIMULATION MODEL

Numerical device simulation is an important procedure for the design and optimization of novel semiconductor devices [22–24]. Advantages are the calculation of the electrical behavior before the fabrication process, the calculation, and visualization of inner-electronic values, which are not measurable. The advanced miniaturization in the semiconductor technology requires an upgrade of conventional simulation models because several quantum mechanical effects like tunneling through potential barriers or particle accumulation in quantum wells appear in these nanometer scaled structures. An important issue in any device simulation is the inclusion of correct material parameters such as band offset, Eigen energy, carrier mobility, and carrier recombination coefficients which are a function of material

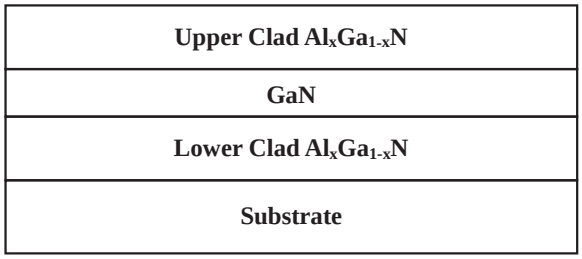

Figure 1. $GaN/Al_xGa_{1-x}N$ based quantum well structure laser diode.

composition [25, 26].

For our simulation we had considered the simple quantum structure as shown in Figure 1. From Figure 1 it is clearly observed that under biased condition the barrier height at the two interfaces are different. To analyze the quantization effect in quantum structure we had solved the Schrödinger equation by using Transfer matrix method. The time independent Schrödinger equation with an electric filed is given as follows

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

where, m^* is the effective mass, h, is the Planck's constant, E, is the Eigen energy

$$V(x) = -|e|\,\phi(x) + V_c(x) + |e|\,Fz \tag{2}$$

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 our calculation. The envelope wavefunction $\psi(x)$ of Schrödinger equation when solved with an appropriate boundary conditions the general solution for quantum well and barrier region obtained are given by Equations (3a) to (3b) as follows.

$$\psi_I(x) = A_1 e^{ik_1 x} + A_2 e^{-ik_1 x} \tag{3a}$$

$$\psi_{II}(x) = B_1 \cos(k_2 x) + iB_2 \sin(k_2 x) \tag{3b}$$

$$\psi_{III}(x) = C_1 e^{ik_1 x} + C_2 e^{-ik_1 x} \tag{3c}$$

The implementation of the transfer matrix method has been carried by applying appropriate boundary conditions. The matrices obtained for the single quantum well structure by considering the wave

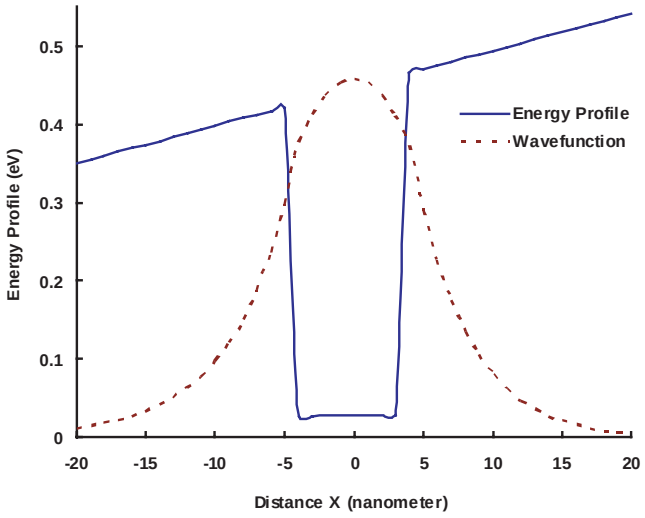

Figure 2. Energy profile and Wavefunction as function of distance X.

function at interface to be equal according to the boundary conditions are as follows.

$$M_1 \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = M_2 \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} \tag{4a}$$

and

$$M_3 \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} = M_4 \begin{bmatrix} C_1 \\ C_2 \end{bmatrix} \tag{4b}$$

While M_1, M_2, M_3, M_4, are given by the following expressions.

$$M_1 = \begin{bmatrix} e^{-k_1 a} & e^{k_1 a} \\ k_1 e^{-ka} & -k_1 e^{ka} \end{bmatrix}, \tag{5a}$$

$$M_2 = \begin{bmatrix} \cos(k_2 a) & -\sin(k_2 a) \\ k_2 \sin(k_2 a) & k_2 \cos(k_2 a) \end{bmatrix} \tag{5b}$$

$$M_3 = \begin{bmatrix} \cos(k_2 a) & \sin(k_2 a) \\ -k_2 \sin(k_2 a) & k_2 \cos(k_2 a) \end{bmatrix} \tag{5c}$$

$$M_4 = \begin{bmatrix} e^{k_1 a} & e^{-k_1 a} \\ k_1 e^{ka} & -k_1 e^{-ka} \end{bmatrix} \tag{5d}$$

Then by further solution we get Equation (6) as given below which is very useful for the determination of the Eigen energy and

transmission coefficient of the quantum well structure based laser diode. The Eigen energy is necessary for the determination of the wave vectors of the quantum well and barrier region. The probability density, confinement factor and other electrical properties, thus the transfer matrix method provides a number of electrical properties efficiently and accurately.

$$\begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = M_1^{-1} M_2 M_3^{-1} M_4 \begin{bmatrix} C_1 \\ C_2 \end{bmatrix} \tag{6}$$

3. RESULTS AND DISCUSSION

There has been great in the high speed modulation of semiconductor laser sources used mainly for large capacity optical communication system. More recent developments include the field induced gain switching of semiconductor lasers. Hence, we tried to carry out the analysis of single quantum well structure Gallium Nitride based laser diode under an applied electric field. The analysis has been carried out for varying well width and different Aluminum mole fraction under biased conditions. We, assumed 5 V potential across the quantum well laser diode.

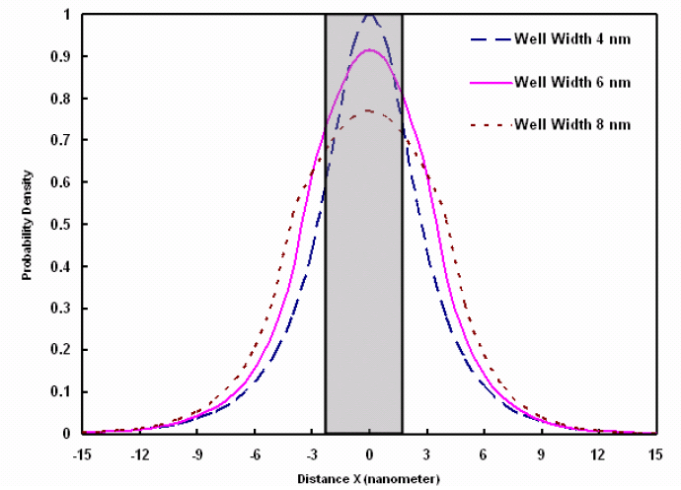

Figure 3. Probability density for varying well width vs distance X.

Figure 3 reveals the electron probability density of finite potential quantum well structure laser diode. The result has been carried out for varying quantum well width and across the whole device length.

From figure it is clearly observed that for the narrower well width the probability has maximum amplitude, while with increase of the well width amplitude decreases. An important observation from Figure 3 is that the wavefunction grows sharply for narrow quantum wells, while for broader well width the wavefunction are not much sharper. The sharpness of the wavefunction for well width of 4 nm is due to the fact that Eigen energy is much higher i.e., 100 meV and above along with the length of the device as observed in Figure 4. The Eigen energy increases almost linear along the X-axis, and decreases with the increase in well width.

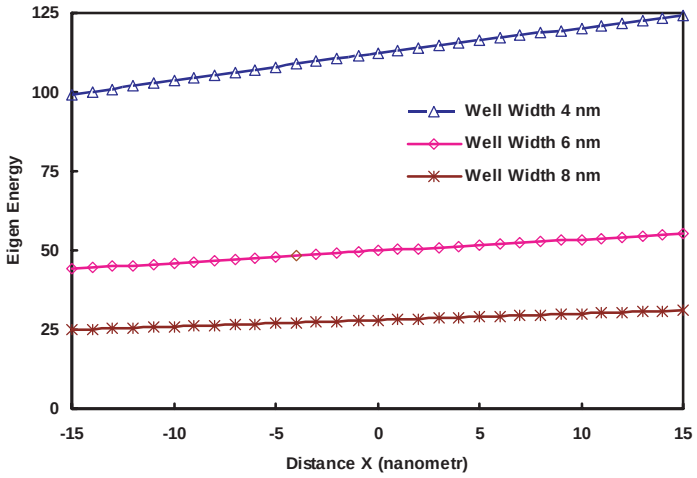

Figure 4. Eigen energy for different well width for corresponding position in quantum structure.

As it is already mention that the material composition is very vital in determination of the electrical and optical properties of the quantum well devices. Hence, we had carried out the wavefunction analysis for the different Aluminum mole fraction. In Figure 5, the amplitude of probability density for Aluminum concentration 10% is much lower and the spread of wavefunction distribution is much more. Since, the barrier height of the quantum well is low results in a greater probability of electron tunneling and hence, the spread of distribution function for lower Aluminum concentration is much greater. In Figure 6 the Eigen energy for different Aluminum concentration is given as a function of distance X. The Eigen energy for Aluminum mole fraction 0.1 varies from 13.69 meV to 58.327 meV. The probability density for 30% Aluminum mole fraction reveals that the electron confinement at higher Eigen energy and barrier height is better. The Figure 7 shows non-

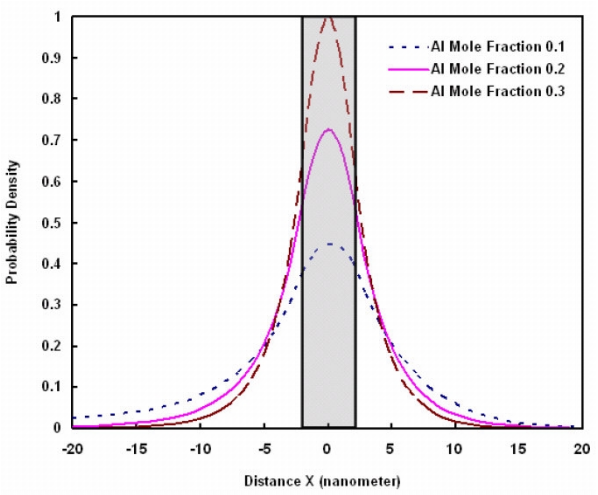

Figure 5. Probability density for varying aluminum concentration vs distance X.

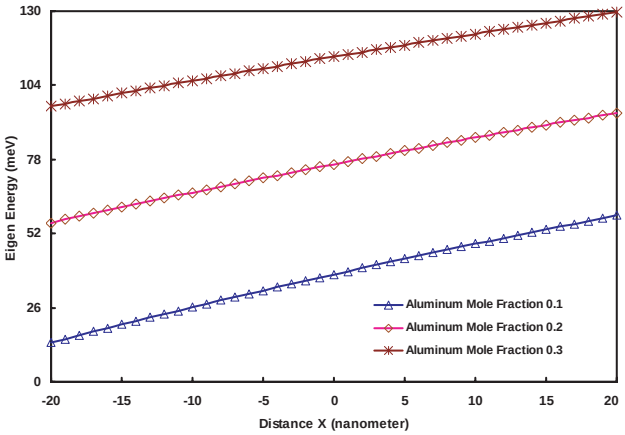

Figure 6. Eigen energy for different aluminum concentration for corresponding position in quantum structure.

linear increment of the FWHM with the increase in quantum well width, while a non-linear decrement for the increase in Aluminum concentration. The increase in well width increases the FWHM from 5.4 nanometer to 9.4 nanometer, while the increase in the Aluminum concentration the FWHM decreases from 8.98 to 5.4.

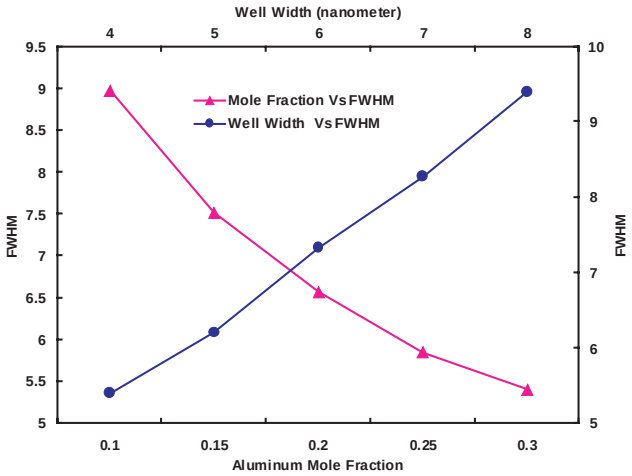

Figure 7. FWHM of the probability density as function of well width and aluminum mole fraction.

4. CONCLUSIONS

The transfer matrix method is faster, accurate, and simpler to implement it for the solution of the Schrödinger equation. The Eigen energy has been deuced for different Aluminum mole fraction and well widths. The Eigen energy variation observed to be from 13.69 meV to 129.38 meV. The applied electric field in the quantum structure causes the variation in the Eigen energy along the X axis shows a vast variation.

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