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Effect of Aluminum mole fraction and well width on the probability density spreading in GaN/AlGaN quantum well

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Here, we modeled a novel equation to determine full width at half maxima (FWHM) of probability density in GaN/AlGaN quantum well structures in order to investigate the effect of aluminum mole fraction and well width on the quantum confinement. Solutions of the Schrodinger's time independent equation have been obtained using Quantum Transmitting Boundary Method (QTBM) and transfer matrix method (TMM) has been used to compute the energy and transmission coefficients. The wave function and probability density have been obtained for single quantum well structure of GaN/AlGaN. The results obtained through our probability density spreading model shows excellent agreement with the analytical results. Our versatile approach explores the probability density spread in terms of FWHM with simultaneous variations in well widths and Aluminum mole fraction x. Our model provides useful physical insight to optimize structural parameters for the better quantum confinement in emerging GaN based quantum well laser diodes.

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1. Introduction

Despite of very extensive applications, electronic devices from Si, GaAs and their alloys are intolerant of elevated temperatures. The wideband gap nitride materials have emerged as strong candidates for electronics and optoelectronics applications since they are potentially free from these shortcomings. These materials are the basis for a number of well-established commercial technologies [1,2] and provide potentials for the expansion of semiconductor technology for numerous applications ranging from outdoor televisions, traffic signals, scanners, flashlights and automotive backlighting. They are very significant in optical storage applications [3-6] because the storage density of optical compact discs (CDs) and DVDs is inversely proportional to the square of the laser wavelength. It is possible to obtain emission in wide range from blue to ultra-violet using GaN. However, to achieve reliable illumination and economical GaN based light emitting devices, intensive research efforts are needed to commercialize them for optical storage, energy efficient lighting, efficient communication and high-resolution printing.

In order to achieve these goals, the researchers have focused their attention on GaN based light emitting devices working in a full color display spectral range. The double heterostructure of GaN provides better optical confinement [7], however, in quantum well structures, the quantization effects drastically modifies the energy spectra of confined electrons. The gain necessary for lasing action occurs more efficiently as the active semiconductor region is scaled down from the bulk to the nanometer scale. Consequently, semiconductor lasers built with quantum nanostructures are expected to exhibit extraordinary features such as high optical gain, great colour range and low lasing threshold. In a quantum well structure, a series of energy levels and associated subbands are formed due to quantization of carriers in the direction of quantum well thickness. The carrier confinement and its resulting density of states in quantum wells promise more efficient lasing devices. When the quantum wells of Gallium Nitride are sandwiched between the $Al_xGa_{1-x}N$ barriers it provides an excellent electron confinement.

The vital parameter in quantum structure based laser diode is transmission coefficient. Hence, analysis of transmission coefficient has been carried out as a function of energy E, which is very useful in determining the tunneling current in quantum well device [8]. The transmission coefficient varies non-linearly with the variation in the energy, where the transmission coefficient, which quantifies the proportion of electron that tunnel through a barrier. Since, the electron wave function penetrates into barrier region due to finite potential depth, it is necessary to optimize the structural and physical parameters for better electron confinement in a quantum well laser diode. The quantum transmitting boundary method (QTBM) [9] provides well-suited approach to explore the electron probability density in the quantum well region by solving the Schrödinger equation.

The energy of the confined carriers depends primarily on quantum well width, as revealed by Gmachl et. al. [10]. They studied the super continuum laser exploring mode

intensity, luminescence power and the electrical characteristics. It was observed that electron probability density depends on the quantum well thickness and effective mass of the carriers of Gallium Nitride and Aluminum Gallium Nitride. The variation in the spreading of electron in the quantum well structure is observed due to the band offset of quantum well and the barrier region.

We present here a model to express probability density spreading in terms of FWHM. The electron energy has been determined through the transcendental equations using an iterative method. We had used transfer matrix method with appropriate boundary conditions and assuming the electron probability density approaches to zero at the edges of quantum well laser diode. The analysis of the probability density and the wave function of the electron were carried out for the different quantum well thickness and Aluminum mole fraction. The results for the probability density and the relative wave function amplitudes are presented in this paper.

We have investigated for the first time a novel equation for the determination of spread of probability density function in the form of FWHM as a function of well width and Aluminum mole fraction x of barrier layer in single quantum well of $GaN/Al_xGa_{1-x}N$. The equation developed allows simultaneous variation of either well width or Aluminum mole fraction x to determine FWHM of probability density exploring the spreading of the probability density. This spreading is very useful to promote the quantum confinement and penetration of wave function in the barrier as a function of well width and Aluminum mole fraction. The following section of the paper explains the mathematical approach used for the modeling and simulation of probability density spreading. The results obtained through our equation have been verified and found to be in excellent agreement with analytical results as speculated in section III of the paper. Finally, section IV highlights the conclusion.

2. Mathematical approach

In order to model the complete carrier transport and capture process, one needs to examine the nature of the confinement and quantum well regions as well as their mutual coupling. The carriers in the quantum wells are confined in one dimension and have discrete energy bands. Here, the square of wave function is interpreted as the amplitude of probability density for realizing the presence of electron particle in a confined region. The Schrödinger equation describes the transportation of the carriers from one state to the other state that leads to continuity and the probability density arise due to the probability current and imaginary part of the potential [11]. As the size of the modern devices is approaching to quantum size, treatments, the particle wave dualism must be applied. Therefore, the Schrödinger equation with a convenient approximation must be used to model the semiconductor quantum heterostructures. This is a delicate approximation since it does not include possibility of propagation outside the structure. Therefore, appropriate boundary conditions must be applied to give the correct physical behavior [12].

We considered the time independent effective mass Schrödinger equation in the one-dimensional varying envelope approximation.

$$\frac{d^2\Psi(x)}{dx^2} = -\frac{2m^*}{\hbar^2}(E-V)\Psi(x) \qquad (1)$$

At this juncture, Ψ(x) is the envelope function, E is the eigen energy and V is band offset between the barrier region and quantum well, and m* is the effective mass.

M. V. Fischetti [13] has suggested that one can obtain the wave function amplitude and reflection/transmission coefficients. Under both the effective mass and envelope function approximations, the alternating layers of dissimilar semiconductors show more relevance for finite quantum well model [14] as shown in Fig. 1.

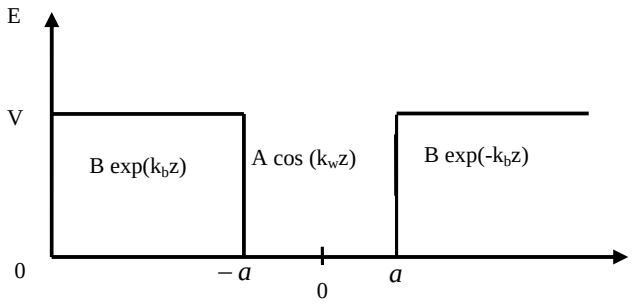


Fig. 1. Finite potential well.

The boundary conditions are imposed to the Schrodinger equation and the general solutions for each layer have been obtained. The general solutions of the Schrodinger's equation using the boundary conditions are as follows:

$$\begin{aligned} \psi(z) &= B\exp(k_b z), \quad z \le -a \\ \psi(z) &= A\cos(k_w z), \quad -a \le z \le a \\ \psi(z) &= B\exp(-k_b z), \quad a \le z \end{aligned} \qquad (2)$$

These general solutions include the arbitrary constants, which are determined through the normalization of the wave function under the specified boundary conditions and perceptive that at the interface the continuity is provided by the wave function [15]. The wave vectors k_w and k_b are given by the following equations and to be determined with a different approach with E is the eigen energy of the particle and V is potential depth.

$$k_w = \frac{\sqrt{2m_w^* E}}{\hbar} \quad \text{and} \quad k_b = \frac{\sqrt{2m_b^*(V-E)}}{\hbar} \qquad (3)$$

In equation (3) m_w^* is electron effective mass in well region of GaN ($0.2m_0$), m_b^* is the electron effective mass of $Al_xGa_{1-x}N$. The following relation can obtain the electron effective mass for barrier region material $Al_xGa_{1-x}N$ with respect to mole fraction.

$$m_e(x) = [0.3x + 0.2(1-x)]m_0$$

k_w and k_b are the wave vectors in a quantum well and barrier region respectively. These, wave vectors have been used to determine energy through an iterative method by yielding first the transcendental equations using the transfer matrix method. The transcendental equations for the odd and the even parity are obtained respectively as

$$k_w \times \tan k_w a = k_b$$
$$k_b \times \tan k_w a = k_w \quad (4)$$

Here, the wave vectors k_w and k_b of the well region and the barrier region respectively are functions of the energy. Thus, energy E is the vital parameter and need to be determined with proper considerations. It was observed that the energy shows great variation with the physical parameters such as well width and barrier height. These parameters are crucial in the study of tunneling current as well and tunneling can be analyzed through transmission coefficients. Hence, we had determined transmission coefficients through the following expression given below. The procedure assumed that all charge carriers approaches in double barrier quantum well structure. The transmission coefficient shows dependence on energy, the well width and the band offset arise due to quantum well heterostructure. The transmission coefficient for energy less than band offset is given as

$$T = \frac{1}{1 + \left(\frac{k_w^2 + k_b^2}{2 k_w k_b} \right)^2 \sinh^2(2 k_b a)} \quad (5)$$

At this juncture, kw and kb are the wave vectors and '2a' is the width of the quantum well. In case of energy greater than band offset, the wave vector of the barrier region kb is given in equation (6) as follows;

$$k_b = \frac{\sqrt{2m^*(E-V)}}{\hbar} \quad (6)$$

The material and physical parameters used for the analysis are listed in Table 1.

Table 1. Physical parameters used for the analysis.

	Barrier Region	Well Region
Material	AlGaN	GaN
Layer Length (nanometer)	28.5	3
	27	6
	25.5	9
Aluminum Mole Fraction	25%	-
Electron Effective Mass	0.225 m_0	0.2 m_0
Band Offset (V)	396 meV	

3. Results and discussion

The energies of carrier are no longer continuous in the confined regions of quantum wells and the discrete states are appeared in nanomaterials. The energy and the wave function are found by solving stationary Schrodinger equation subject to the boundary conditions. Here, we had considered the device length of 60-nanometer, the 25% of Aluminum mole fraction x has been considered, so that the stark effect which emerges with an increase in Aluminum mole fraction due to which the red shift occurs. The analysis of the wave function for different quantum well widths has been carried out. The confinement of wave function in a well region depends strongly on the chosen potential depth due to the band offset developed between the well and barrier region. The potential depth depends on x of the alloy $Al_xGa_{1-x}N$ used for the barrier region. The confinement energy for a finite quantum well was observed to be lower as compared to the confinement energy in an infinite quantum well. The wave function tunnels into the barrier region due to finite potential quantum well as it is demonstrated in Fig. 2. It reveals that the wave function has better confinement for the lower well width than higher values of well widths. This has been attributed to variation in the energy, which affects on the wave vectors kw and kb of the well region and the barrier region respectively. The effect is similar as we observed for the quantum confined stark effect (QCSE) [16] with spatial variance, where the QCSE occurs for the electric field. The variation of wave function shows peak value at the center of the quantum well due to the symmetric quantum well structure.

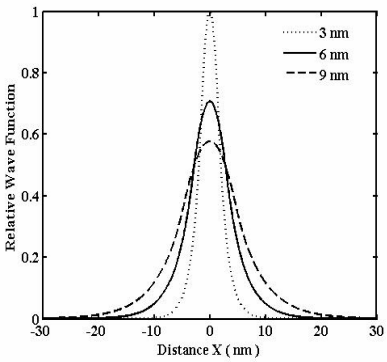


Fig. 2. Wave functions for different well widths.

It has been observed from Fig. 3 that for narrower well, the confinement is more and the spread in probability density reduces with the decrease in well width. Here, the energy E for well width of 3-nanometer was found to be 404 meV, which reduces to 45 meV for the well width of 9-nanometer while the potential V is kept constant at 395 meV. The confinement of the carrier shows dependence on well width and Aluminum mole fraction as the higher band offset achieved with the increase in mole fraction x. The well width and x affects the energy E that results in tunneling from the well to barrier.

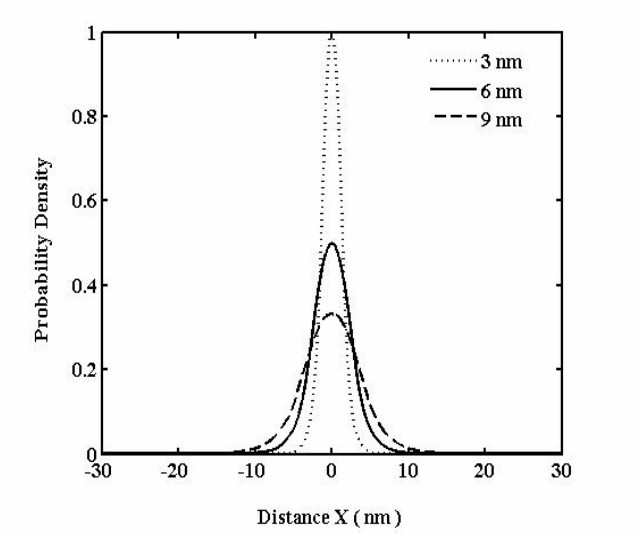


Fig. 3. Probability density variations with distance X.

The tunneling effect can be analyzed through the transmission coefficients. At the interface between the classical and quantum zones, the boundary conditions for the Boltzmann equation depend on the transmission coefficients of the Schrodinger solutions. The determination of the transmission coefficients for Eigen functions through Schrodinger equation for the range of energy permits us to reduce the region of search. Hence, we had analyzed the transmission coefficients for the well width variation for the constant Aluminum mole fraction of 25%. The transmission coefficients for different well widths are depicted in Fig. 4. The transmission coefficient for well width of 3-nanometer reaches to its peak value of 0.903 for the energy value of 1000 meV and for the well width of 9-nanometer it reaches to its peak value of 0.999 with lower energy value of 574 meV. Therefore, it is significant that tunneling is more in case of wider wells, which can be clearly confirmed through the results of the wave function and the probability density. The oscillatory nature of transmission coefficients is observed for greater well widths. These oscillations of transmission coefficient reveal that the energy of carrier is having greater value than the band offset and it leads to complex values.

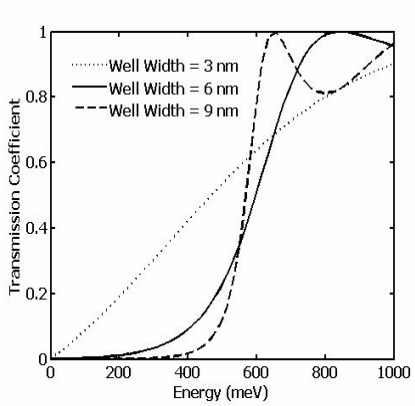
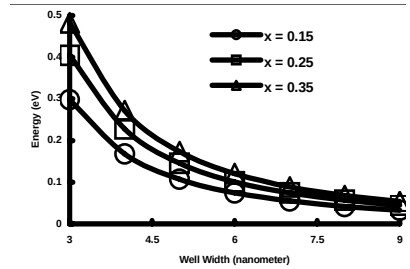
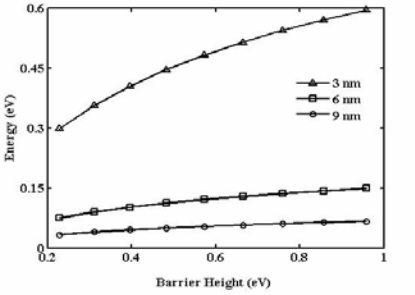


Fig. 4. Transmission Coefficients as function of energy.

It was observed that the Aluminum mole fraction and the well width play a vital role in a physical behavior of the carrier wave function in the quantum well structure. So it is necessary to investigate particularly the effect of well width on the energy of particle in the well region. The Fig. 5(a) and 5(b) shows the electron ground state energy calculated with a constant GaN effective mass. Fig. 5 shows that energy decreases with the increase of well widths and decreases with increase of barrier height. The values of energy obtained for 35% of Aluminum mole fraction are relatively greater than 15% and 25%. The electron energy for the Aluminum mole fraction of 25% varies from 145 meV to 45 meV for different well widths. The higher values of energies are obtained for 3 nanometer well width and show a continuous increase with variation of barrier height. Therefore, for the purpose of optimization and to develop the quantum well lasers diode well width and mole fraction are the most important parameters.



a)



b)

Fig. 5. Variation of energy with a) well width b) barrier height.

Full width at half maximum (FWHM) of probability density has been investigated thoroughly to analyze the behavior of the carrier in the quantum well structure. The simultaneous study of well width and the Aluminum mole fraction through the wave function and probability density is complex. The analysis of these parameters can be comfortably understood through the investigation of FWHM of probability density. The investigation of the FWHM of probability density has been carried out in a very comprehensive manner. It is very clear from our results that better confinement is obtained for the higher mole fraction and lower well width. Particularly, for the aluminum fraction having a value less than 6% the spread of probability density for all the well widths has been observed to be very high revealing that the quantum confinement for such low value of x is immensely poor. We have developed a novel equation to determine spread of probability density in terms of FWHM Ψ_f as a function of well width W and Aluminum mole fraction x as

$$\Psi_f = W(x^3 + 7.305 * x^2 - 4.69 * x + 1.55 + 0.205 * (1.05 + (0.0025 * \frac{(x+1.005)}{x^2}))); \quad (7)$$

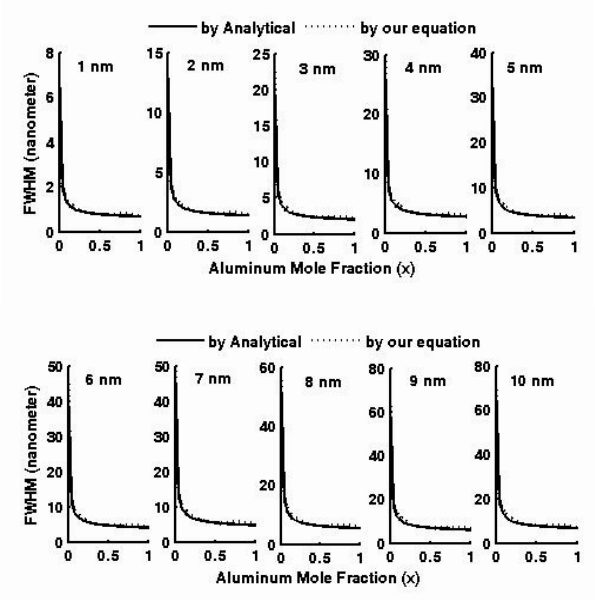


Fig. 6. FWHM of probability density obtained using theoretical analysis and our equation as a function of Aluminum mole fraction x.

Efficient and simple approach has been used to determine spread of probability density in terms of FWHM as a function of W and x. The above equation has been investigated by obtaining the FWHM of the probability density for all the values of x from 1% to 100% and W from 1 nanometer to 10 nanometers in an analytical manner. The FWHM of the probability density obtained through theoretical analytical approach and calculated through our equation (7) have been illustrated in Fig. 6 and Fig. 7. The variation of FWHM with mole fraction x for varying values of well widths from 1 to 10 nanometer was observed to be nonlinear. The spread was found to be greater for lower values of x due to less values of barrier height and band offsets. The linear variation of FWHM with well widths for different values of x was observed due to variations in energy and wave vectors. The solid line shows FWHM deduced through theoretical analysis and dotted line shows results obtained using our proposed equation (7). The results obtained through our equation shows excellent agreement with theoretical results.

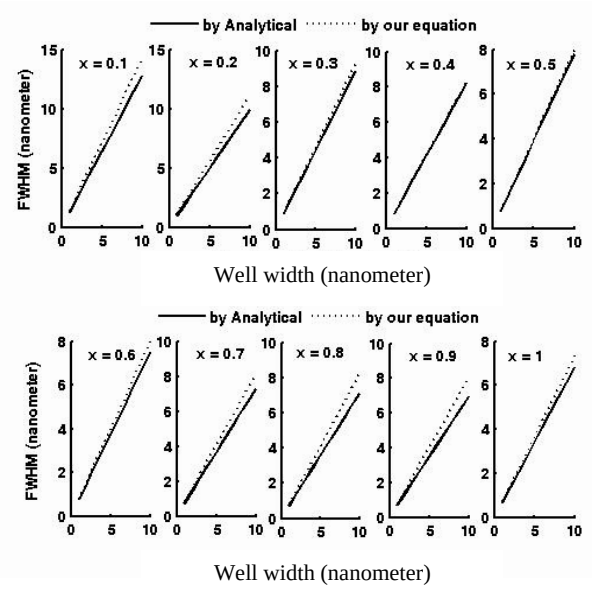


Fig. 7. FWHM of probability density obtained using theoretical analysis and our equation as a function of well width.

4. Conclusion

In conclusion, we proposed a novel approach to determine probability density spread in GaN/AlGaN quantum well structures which allows simultaneous variations of well widths and mole fraction x. Our equation modeled the values of well width and aluminum mole fraction in the barrier region for the nitride based quantum well laser diode structures, efficiently, without solving tedious Schrödinger's equation. We have carried out detailed analysis to obtain wave function, probability density, transmission coefficients and energy to explore carrier transport mechanism in emerging GaN/AlGaN quantum well laser diodes. Furthermore, our analysis provides useful physical insight to optimize physical and structural parameters of GaN/AlGaN quantum well for its better quantum confinement.

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