OPTOELECTRONICS AND ADVANCED MATERIALS – RAPID COMMUNICATIONS Vol. 1, No. 12, December 2007, p. 693 - 697

Quantum confinement and electron capture analysis in GaN multiple quantum well structures

K. TALELE, D. S. PATIL*
Department of Electronics, North Maharashtra University, Jalgaon [Maharashtra], India

Quantum confinement and electron capture analysis have been carried out to enhance the performance of GaN multiple quantum well structures through the optimization of physical, structural and material parameters. Self-consistent convergence of eigen energy has been achieved to have its accurate value for varying aluminum mole fractions in the AlGaN barrier regions. Solutions of the wave function intensity have been obtained using quantum transmitting boundary method and transfer matrix method. The confinement factor was deduced to be 0.8681 for 30% aluminum mole fraction where as for 5% Aluminum concentration it was found to be 0.5435. The oscillatory nature of electron capture time with change of Aluminum mole fraction has been explored using standard Fermi Golden rule based calculations. It is inferred from our analysis that aluminum material composition of barrier strongly affects the quantum confinement.

(Received October 25, 2007; accepted November 22, 2007)

Keywords: Quantum confinement. GaN, Multiple quantum well

1. Introduction

The physics of semiconductor nano-devices, in particular multiple quantum well (MQW) lasers, is influenced significantly by the transportation phenomena of electrons within multiple quantum well heterostructures [1]. The electron confinement and scattering rates of electrons due to optical phonon emission have special significance for studying the optical and electrical properties in such structures [2]. It has thus been realized that accurate modeling of complex quantum structure laser diodes is very crucial to reduce the research time, cost and to achieve better efficiency.

Several, conventional and non-conventional structures have been proposed for investigating peculiar aspects of the confined carrier physics to improve the performance of the multiple quantum well laser diodes [3-4]. The electrical parameters show great dependence on electron and holes interaction within the quantum well region and barrier. Hence, it is very necessary to optimize physical parameters for achieving better output characteristics such as electron capture rate, quantum efficiency, power consumption and threshold current. As compared to the heterostructures, the multiple quantum well provides higher optical gain at lower threshold current which is the elementary reason for the fabrication a quantum well laser diodes. Here, the nanometer thickness of quantum wells has a lower binding energy which endorses better execution of quantum well laser diodes.

The binding energy in the III-nitride semiconductor materials arises from the nitrogen atoms, which have high electron affinity and results in valence charge density well localized in such materials. The gallium nitride (GaN) semi-conducting material has incredible electrical properties such as high electron affinity, high electron mobility and lower effective mass which confer a boost to comprehend an efficient quantum well laser diodes. Therefore, researchers and scientists paid a remarkable interest in III-V nitride based semiconductors because of their immense potential applications in microelectronics and optoelectronics devices [5]. These devices are intended to fulfill the growing demands for high power and high frequency electronic components [6]. Quantum confinement and electron capture play a prominent role to enhance the performance of light emitting devices. The analysis becomes complex as the number of layers in multiple quantum well increases.

Here, we present the electron transport behavior in GaN multiple quantum well structure for the investigation of the quantum confinement and electron capture time. The study of various properties like energy and scattering rate has been carried out by developing the simulation tools using MATLAB software. To realize the complete electron transport phenomena we have utilized the quasi transmitting boundary method (QTBM) and transfer matrix method.

The paper is organized in three main sections. Section 2 is a theoretical analysis in detail. The significant results have been discussed in section 3. Finally, the paper is concluded by highlighting the implications of this work.

2. Theoretical analysis

In this paper, we had considered a planar structure of a multiple quantum well laser diode as shown in Fig. 1(a). The wave function of the quantum well structure was obtained by numerical solution of the effective mass Schrödinger equation [7-9]. The physical parameters like effective mass, barrier height and aluminum mole fraction strongly affects the behavior of the energy levels within the quantum wells. The band offset due to the barrier height plays a significant role in quantum confinement. For the finite quantum well structure, it is considered that the barrier height should be always greater than eigen energy which makes possible the electron confinement. The time independent Schrödinger equation describing

spatial behavior of electron Ψ(x) is given in equation (1). In the well region, conduction band potential 'V' is assumed to be zero and m* is effective mass of Gallium Nitride, where as in the barrier region conduction band potential is 'V' and m* is effective mass of $Al_xGa_{1-x}N$.

$$\frac{\partial^2}{\partial x^2}\psi(x) = \frac{2m^*}{\hbar^2}(V - E)\psi(x) \qquad (1)$$

For solving this equation and to obtain solutions to the wave functions the boundary conditions are used. First and second boundary conditions are that Ψ and ∂Ψ/∂x must be continuous. For finding out the related arbitrary constants to each well and barrier equations, the normalization condition has to be used. The general solutions Ψ(x) of the Schrödinger equation for the barrier region and quantum well region of triple quantum well structure are given below.

$$\begin{aligned}
&\psi(x) = A_1 \exp(qx) + B_1 \exp(-qx), && x < 0\\
&\psi(x) = A_2 \sin(kx) + B_2 \cos(kx), && 0 < x < a\\
&\psi(x) = A_3 \exp(qx) + B_3 \exp(-qx), && a < x < b\\
&\psi(x) = A_4 \sin(kx) + B_4 \cos(kx), && b < x < c\\
&\psi(x) = A_5 \exp(qx) + B_5 \exp(-qx), && c < x < d\\
&\psi(x) = A_6 \sin(kx) + B_6 \cos(kx), && d < x < e\\
&\psi(x) = A_7 \exp(qx) + B_7 \exp(-qx), && e < x < f
\end{aligned} \qquad (2)$$

The solutions of Schrödinger equation confers wave vectors of quantum well and barrier region. The wave vectors k and q are the functions of the energy as shown in the following equations.

$$k = \frac{\sqrt{2m^* E}}{\hbar}, \quad \text{and} \quad q = \frac{\sqrt{2m^*(V - E)}}{\hbar} \qquad (3)$$

Equation (2) shows the general solutions of Schrödinger equation for barrier and well region for triple quantum well structure in which A_i and B_i are arbitrary constants with i = 1 to 7. The q and k are the wave vectors of the barrier region and well region respectively. The wave vectors are obtained from expression (3). The wave vectors k, q and eigenenergy are determined by iterative method and the transfer matrix method. In transfer matrix method, all the matrices are combined in such a way that the coefficient of outer regions is linked. The matrices which are used for the solution of eigenenergy are useful for calculating the transmission Coefficients. The reduced product of these matrices is 2 × 2 matrix which is given by the following equation,

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = M \begin{pmatrix} A_7 \\ B_7 \end{pmatrix} \qquad (4)$$

where, M is product of all the matrices obtained through the coefficients of arbitrary constant of the general solutions of the Schrödinger equation in each layer of the quantum well structure by applying a boundary conditions as mentioned earlier. The suffix n denotes the top most layer of the quantum well structure. Then one can obtained the arbitrary constant by converting the 2×2 matrix in the form of an expression as follows.

$$\begin{aligned}
A_1 &= M_{11}A_7 + M_{12}B_7\\
B_1 &= M_{21}A_7 + M_{22}B_7
\end{aligned} \qquad (5)$$

The probability interpretation of the wave function implies that the wave function must tend towards zero into the outer barriers, i.e. the coefficients of the growing exponentials must be zero. Therefore, at the first and last interface, B_1=0 and A_7 =0, and hence in the above equation we gets M_{22} = 0, since B_7 cannot be zero. As all of the elements of M are function of the k and q, which are again the function of the energy E, they have to satisfy the condition $M_{22}(E) = 0$. Once the energy is known, the coefficients A_7 to B_7 are determined and the envelope wave function can be deduced.

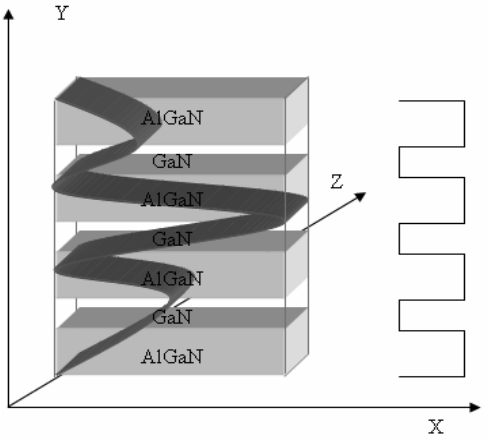


Fig. 1(a). $GaN/Al_xGa_{1-x}N$ based Multiple Quantum Well Structure.

The Schrödinger equation provides the basis to realize the quantization effect and very useful to optimize the structural and electrical parameters of quantum well structures. The confinement of electron in the well region and its recombination plays a vital role in enhancing the optical gain and quantum efficiency. Hence, it becomes necessary to investigate electron capture time within the well region. The electron capture time shows a great dependence on aluminum mole fraction [10-12]. The following equation (6) has been realized through the standard calculations of Fermi golden rule. The electron capture rate, shows the dependence on material and electrical parameters such as static dielectric constant, kinetic energy and barrier height. These parameters are the functions of the aluminum mole fraction and hence we have studied the dependence of the electron capture time on aluminum material composition in the barrier.

$$\frac{1}{\tau} = \frac{e^2 \omega_L m_w}{8\pi\hbar^2}\left(\frac{1}{k_\infty} - \frac{1}{k_s}\right)\int_0^{2\pi} d\theta \frac{F_q}{q}$$

$$q = \frac{\sqrt{2m}}{\hbar}\left[2E - V - 2E^{1/2}(E+V)^{1/2}\cos\theta\right]^{1/2} \quad (6)$$

$$F_q = \int_{-\infty}^{\infty} \psi_x' e^{-qx} \psi_x dx$$

At this juncture, ω_L is the phonon frequency, m_w is the mass of GaN, k_s and k_∞ are the static and dynamic permittivities, F_q is the form factor which provides the information about the relative strength of the dielectric carrier transitions [13,14].

3. Results and discussion

For developing the efficient laser diodes, it is important to study the effect of different types of physical, electrical and material parameters. The aluminum mole fraction is one of the most significant parameters to study the electrical and optical characteristics of the multiple quantum well laser diode structure.

The wave function intensity of triple quantum well structure is shown in Fig. 1(b) with variations in aluminum mole fraction. We found that the wave function intensity increases as the aluminum mole fraction increases. The result shows the oscillatory nature of wave function intensity due to the solutions of Schrödinger equation consisting of growing and decaying terms. The increase in wave function intensity in well region has been attributed to the band offset between well and barrier region. The aluminum mole fraction has been increased from 5% to 30%, and the corresponding eigenenergies are deduced from our calculations which are given in Table 1.

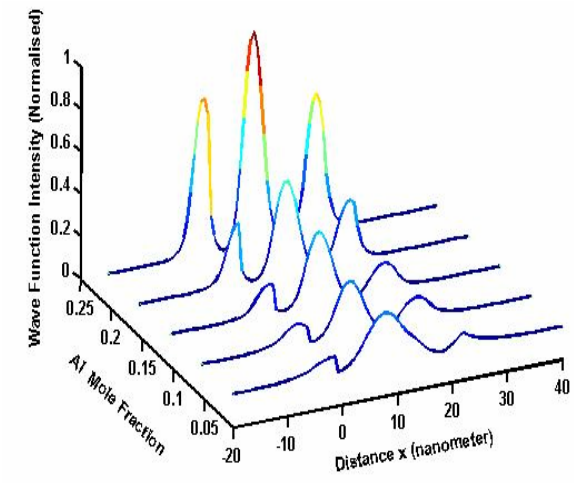
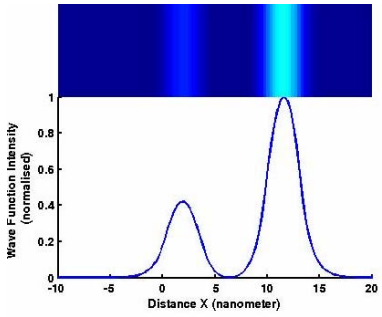


Fig. 1(b). Wave function intensity as a function of aluminum mole fraction in 3 well structures.

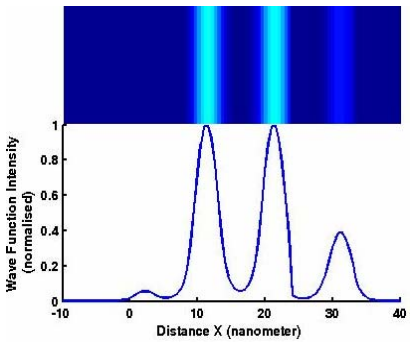
Table 1. Physical, Structural and Material parameters of Triple Quantum Well Structure.

Aluminum mole (fraction)	Barrier width (nanometer)	Well width (nanometer)	Energy (eV)	Barrier height (eV)
0.05	10,4.6,2.1,10	4, 6.9 ,9.3	0.0494	0.0738
0.1	10, 5.2, 5.8, 10	3.5, 5.5, 6	0.0965	0.1503
0.15	10, 5.1, 5.2, 10	3.5, 6.2, 5	0.1060	0.2294
0.2	10, 5.25, 6, 10	3.4, 5.35, 4	0.1236	0.3112
0.25	10, 5.84, 6.6, 10	3.2, 4.46, 3	0.1949	0.3956
0.3	10, 5.13, 5.7 10	4, 4.37, 4.3	0.2163	0.4827

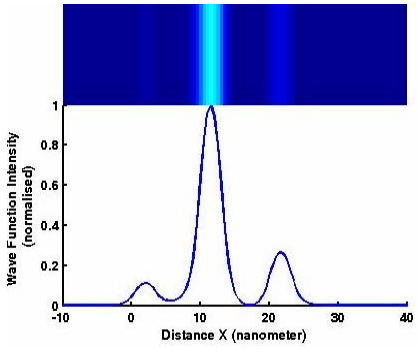
Fig. 2 shows the wave function intensity for the varying number of layers of quantum well structure with their surface images. For the odd number of layers, the electron confinement is in the centre of the whole structure whereas in the four quantum well structure, we can find the quantum confinement in the middle of two quantum well regions and in two quantum well structure it is in second quantum well. For analysis of these results the aluminum mole fraction was considered to be 30%, while the barrier height and barrier mass were estimated to be 0.4827 eV and 2.5844×10^{-31} Kg respectively. Furthermore, it revealed from our analysis that the eigen energy varies according to the variation of structural parameters like well width and barrier width.



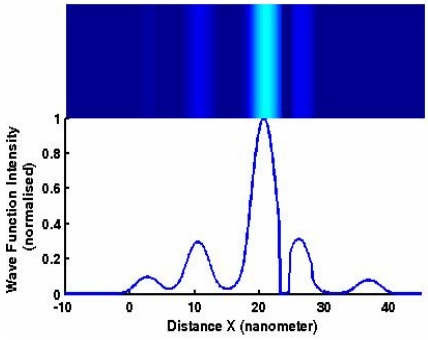
(a)



(b)



(c)



(d)

Fig. 2. Wave function intensities and surface images in 2, 3, 4 and 5 well structures.

The computational efforts needed for the self-consistent convergence of eigen energy in triple quantum well structure for the different values of aluminum mole fraction has been investigated in Fig. 3. It is clear that the execution time required is more for the higher values of Aluminum mole fraction whereas it is less for the lower concentration of aluminum. The execution time was predicted to increase from 0.3906 seconds to 0.4847 seconds for the corresponding increase in aluminum mole fraction from 5% to 30% respectively. This increase of execution time with aluminum mole fraction has been ascribed to the higher number of iterations required to obtain accurate eigen energy value for higher band offset.

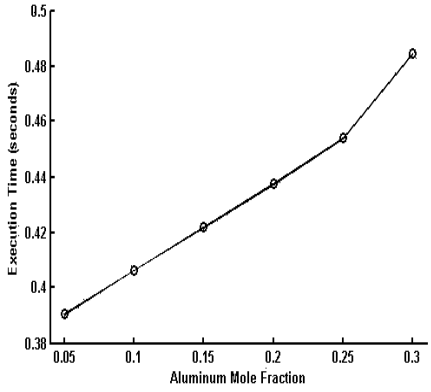


Fig. 3. Execution time needed for self-convergence of eigen energy.

It has been observed from Fig. 4 that with increase in the number of wells, the eigenenergy value decreases. In multiple quantum well structure, as number of wells and barriers increases, the eigenenergy decreases as energy get reduced due to increase in the dimensions of the device. The eigenenergy values were found to decrease from 0.2427 eV to 0.1691eV as number of wells increased from 2 to 5. Here, the constant barrier height of 482.7 meV was attained for the 30 % Aluminum concentration. The spread of wave function intensity has been explored to account for the quantum confinement in multiple quantum well structures as illustrated in Fig. 5. Full width of half maximum (FWHM) of the wave function intensity was found to be decreasing with the increase in aluminum mole fraction. The FWHM of wave function intensity in the central well shows its extension within barrier regions and it has been realized that the electron transmission in barrier region is more for lower band offset. Hence, the intensity spread was found to be decreased from 7.5 nm to 3.5 nm for the aluminum concentration change of 5% to 30%. This non linear decrease in the spread of wave function intensity is due to the increase in the barrier height at the $GaN/Al_xGa_{1-x}N$ interface.

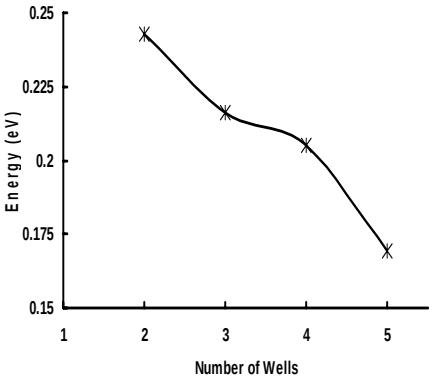


Fig. 4. Eigen Energy as a function of number of wells (maximum 5).

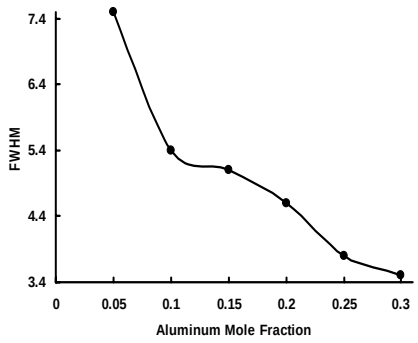


Fig. 5. Full Width Half Maxima of wave function intensity.

The quantum well structure provides a better electron confinement within the well region. The enhanced accumulation of the electrons with the increase in band offset is expected and it is clearly observed in Fig. 6. The

quantum confinement factor was found to be increase with increase in Aluminum mole fraction. The confinement factor was worked out to be 0.8681 for 30% aluminum mole fraction where as for 5% Aluminum concentration it was found to be decreased to 0.5435. The confinement factor demonstrates the quantum confinement which increases exponentially with the increase in mole fraction. Here, we had restricted ourselves to obtain the quantum confinement up to 30% of Aluminum mole fraction only as the value of confinement factor saturates for higher Aluminum mole fractions.

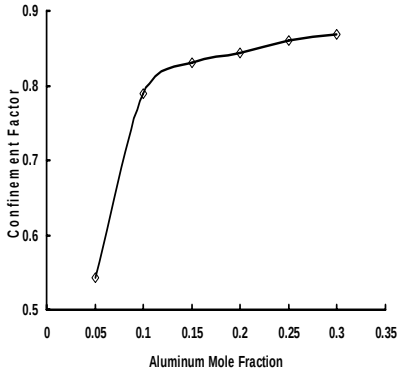


Fig. 6. Quantum confinement as a function of aluminum mole fraction.

The one dimensional quantum structure restricts the electron to be transmitted in the barrier region. Hence, the electron present in the well region generates the electron hole pair and thus spontaneous emission arises due the population inversion. This recombination rate is highly dependent on the electron capture time. The electron capture time as a function of the Aluminum mole fraction has been explored as shown in Fig. 7. The oscillatory nature is obtained due to the material and structural properties [15-16]. It reveals from our analysis that the minimum capture time was 2.2368 ps for 0.1 concentration of Aluminum while, the maximum value attained was 9.4317 ps for 0.2 Aluminum mole fraction. This variation in electron capture time is attributed to the continuum bound state in the well region which has the higher electron probability density.

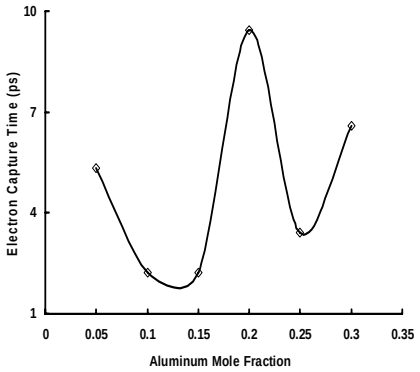


Fig. 7. Electron Capture Analysis in multiple Quantum well structures.

4. Conclusions

The GaN multiple quantum well structure is analyzed for its quantum confinement and electron capture mechanism. Effect of Aluminum mole fraction on the quantum confinement and electron capture time has been explored. The behavior of wave function intensity spread as a function of well width and number of wells have been considered. The wave function intensity varies with the change in the aluminum mole fraction due to alteration in the eigenenergy and barrier height. The mighty peak of wave function intensity and bright band in surface image clearly shows the confinement in the innermost quantum well of the device. The quantum confinement of electron in the well region and its recombination plays a vital role in enhancing the optical gain and quantum efficiency.

References

[1] V. N. Sokolov, K. W. Kima, V. A. Kochelap, D. L. Woolard, Journal of Applied Physics **96**, 6492 (2004).
[2] P. W. M. Blom, R. F. Mols, J. E. M. Haverkort, M. R. Leys, J. H. Wolter, Superlattices and Microstructures **7,** 319 (1990).
[3] W. Feng, J. Q. Pan, L. Wang, Z. Y. Liao, Y. B. Cheng, D. B. Chen, L. J. Zhao, H. L. Zhu, W. Wang, Semiconductor Science Technology **22,** 859 (2007).
[4] S. Khatsevich, D. H. Rich, S. Keller, S. P. DenBaars, Physical Review B **75**, 035324 (2007).
[5] D. Gregušova1, R. Stoklas1, K. Cico1, T. Lalinsky1, P. Kordo1, Semicond. Sci. Technol. **22**, 947 (2007).
[6] S.-C. Lee, A. Wacker, Physical Review B **66**, 245314 (2002).
[7] E. P. Samuel, K. Talele, U. Zope, D. S. Patil, Optoelectron. Adv. Mater. – Rapid Communications **1**, 221 (2007).
[8] Erik L. Waldron, E. Fred Schubert, Physical Review B **67**, 045327 (2003).
[9] Juan A. Monsoriu, Francisco R. Villatoro, Marıa J. Marın, Javier F. Urchueguıa, Pedro Fernandez de Cordoba, Eur. J. Phys. **26,** 603 (2005).
[10] Stavrou, Bennett, Al-Dossary, Babiker, Physical Review B **63,** 205304 (2001).
[11] Chin-Yi Tsai. Lester F. Eastman, Yu-Hwa Lo, Chin-Yao Tsaj, IEEE Photonics Technology Letters **6**, 1088 (1994).
[12] P. W. M. Blom, R. F. Mols, J. E. M. Haverkort, M. R. Leys, J. H. Wolter, Superlattices and Microstructures **7,** 319 (1990).
[13] Martin Mosko, Karol Kalna, Semicond. Sci. Technol. **14**, 790 (1999).
[14] Karol Kalna, Martin Mosko, Physical Review B **54**, 17730 (1996).
[15] K. Muraki, A. Fujiwara, S. Fukatsu, Y. Shiraki, Physical Review B, **53**, 15477 (1996).
[16] G. C. Crow, R. A. Abram, Semicond. Sci. Technol. **14,** 1 (1999).

*Corresponding author: patildsp@rediffmail.com