OPTOELECTRONICS AND ADVANCED MATERIALS – RAPID COMMUNICATIONS Vol. 1, No. 5, May 2007, p. 221 - 226

Semi-classical analysis of hole capture in Gallium Nitride quantum wells

E. P. SAMUEL, K. TALELE, U. ZOPE, D. S. PATIL*
Department of Electronics, North Maharashtra University, Jalgaon [Maharashtra], India

Semi-classical theoretical analysis of hole capture in a Gallium Nitride quantum wells has been carried out with hole-optical phonon scattering mechanism. Our analysis shows that the hole capture time varies as a function of the excess energy, quantum well width, barrier width and aluminum (Al) mole fraction in the barrier layer. Strong dependence of hole capture time on mole fraction x in the barrier layer of $Al_xGa_{1-x}N$ has been attributed to the variation of energy and barrier height. Scattering rate due to hole-optical phonon as a function of narrow quantum well width seems to oscillate for different values of Al mole fraction increasing to a very high value with the increase of quantum well width. The energy distribution function for holes reveals nonlinear change with energy. The hole capture time was deduced to be varying from 0.3 ps to 65 ps with variation of structural parameters of the quantum well and Al mole fraction in the barrier.

(Received February 21, 2007; after revision March 17, 2007; accepted April 5, 2007)

Keywords: Gallium Nitride, Hole Capture, Optical phonon scattering, Quantum well

1. Introduction

A new cutting-edge class of electronic and optoelectronic devices has emerged to a great extent due to III-V semiconductor compounds. Specifically, GaN and AlGaN are the basis for a number of well-established commercial technologies due to their large electron and saturation velocity, high thermal stability and large band gap which make them ideal candidates for high power, high temperature and high frequency electronic applications like laser diodes, light emitting diodes, electro-optic modulators, high electron mobility transistor (HEMT) and heterostructure bipolar transistors [1-5].

Quantum Well (QW) lasers are expected to exhibit superior lasing properties such as lower threshold current density and higher differential gain as compared to heterostructure laser diodes. Thus, optical transitions in near surface quantum wells offer the possibility to study the influence of the surface on the quantum well eigenstates. The interaction between carriers confined within the well region and surface states can be controlled by the variation of the quantum well width, thickness of the top barrier layer and the potential depth. The lasers based on GaN/AlGaN quantum wells emit light in a wide range of wavelengths [6-7].

The wave function of a narrow quantum well with high quantization energy penetrates deeply into surrounding barrier material and therefore is very sensitive to influences of the surfaces [8]. In contrast, carriers in a wide quantum well are mainly confined within the active well region resulting in a low sensitivity for surface related disturbances. Therefore, quantum well heterostructures are of great research interest in the recent years particularly due to very short escape time of the carriers [9-14]. The carrier tunneling between adjacent quantum wells modifies the recombination kinetics and transport properties eventually leading to mini-band formation in periodic structures [15]. In case of thick barriers, the dipole-dipole interaction has been investigated as an important mechanism for the population transfer among different wells, both in the Stokes and anti-Stokes directions [16]. Infrequent efforts have been made to explore the significance of the carrier capture in quantum well structures and as a consequence very few comparable values are available [17].

Calculating the carrier capture time by the quantum well involves the computation of the probability per unit time that a carrier in some initial state in quantum well heterostructure emits a longitudinal optical (LO) phonon and ends up in some final state within the quantum well as dictated by energy and momentum conservation conditions. In addition the capture time of electron and hole in the quantum well shows great significance in the lasing action and needs the attention for the improvement of the laser diode efficiency to lower the threshold current [18]. Hence, it was thought that it is necessary to put emphasis on theoretical studies concerning the process of carrier capture within a quantum well. They have been carried out using different models, e.g. emission of optical phonons or carrier-carrier scattering in a layered system [19-20]. Capture of carriers into quantum wells has been studied with considerable interest aimed at optimizing efficiency for improved performance of quantum well lasers and fast switching action. Here, we present analysis of hole capture time and its dependence on mole fraction, excess energy and barrier width.

The main goal of the paper is to investigate hole capture time and scattering rate and their dependence on physical and structural parameters of the GaN/AlGaN quantum well to optimize the performance and enhance the efficiency of GaN based quantum well lasers. Present work explores the phenomena of hole capture in quantum well region of GaN for different Aluminum mole fraction in AlGaN, which is used as a barrier region. The results obtained for the hole capture with respect to barrier width agree with theoretical results of Lingk et.al. [21]. The essential results of scattering rates have been deduced through quantum mechanical model. The scattering rate has been obtained by solving first the Schrödinger equation for which we had used quantum transmitting boundary method (QTBM) originally developed by Lent and Kirkner in 1990 [22]. The semi-classical model used for our analysis provides useful physical insight of carrier transport and hole capture within the quantum well. Section 2 of the paper describes theoretical model and analysis of hole capture. The results of hole capture and scattering phenomena are discussed in section 3 and conclusions are highlighted in section 4 of the paper.

2. Theoretical model

The interactions of hole with the optical phonons in quantum wells and superlattices are of crucial importance in the physics of semiconductor heterostructures. In particular, the intersubband and intrasubband scattering rates for electrons and holes by emission of optical phonons have special significance for studying the optical and electrical properties in such structures. It has thus been realized that accurate modeling of devices such as hot-electron transistors, quantum well laser structures, and infrared detectors requires these scattering rates to be well described. Several Classical carrier transport models are not realistic and sufficient to describe quantum transport of the carriers. Therefore, it is imperative to derive nano-scale quantum mechanical transport model. In order to model the complete carrier transport and capture process, one needs to examine the nature of confinement in quantum well regions. Here, we wish to show the agreement is fortuitous and in fact obscures a much more complicated nature of the hole capture process. We present here, theoretical study for the hole capture time, scattering rate and energy distribution function. The analysis is carried out for the shallow quantum well GaN based laser diode as shown in Fig. 1. Very thin semiconductor film (few nanometers) having optical phonon energy greater than effective barrier height is known as shallow quantum well. The figure shows the potential well with a potential depth of V having dependence on Aluminum mole fraction. The three regions have different solutions obtained through time independent Schrödinger equation described below in equation (1) and its general solutions obtained by imposing the boundary conditions for the barrier and the well regions are given in equation (2).

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

$$\psi_b(z) = B\exp(k_b z), \qquad -w_1 < z < -\frac{w}{2}$$

$$\psi_w(z) = A\cos(k_w z), \qquad -\frac{w}{2} < z < \frac{w}{2} \tag{2}$$

$$\psi_b(z) = B\exp(-k_b z), \qquad \frac{w}{2} < z < w_2$$

The variables k_w and k_b are the wave vectors given by equation (3) of quantum well and barrier region respectively. To determine the values of these wave vectors the transcendental equations has to be solved through an iterative method. The transcendental equations have been obtained by applying the transfer matrix method to the general solutions of Schrödinger equations using appropriate boundary conditions. The A and B are arbitrary constants deduced by using the boundary conditions and applying the normalization of the wave function. In the following equations the m_w is the effective mass of the GaN material and m_b is the effective mass of $Al_xGa_{1-x}N$ which plays a vital role in determining the energy.

$$k_w = \frac{\sqrt{2m_w^* E}}{\hbar}$$

$$k_b = \frac{\sqrt{2m_b^*(V-E)}}{\hbar} \tag{3}$$

When holes or electrons are confined in regions smaller than a few tens of nanometer, quantum effects become noticeable and the material composition as well as dimensions governs the properties of a structure. Thus, hole and electron capture process is much difficult to understand in a quantum well structure, which enforced us to employ the classical model along with the quantum transport model to realize the comprehensive hole capture phenomena in shallow quantum well. Under the collision-free hole transport conditions, the thermionic emission current fills the quantum well. If the hole mean free path ‘l’, due to the polar optical phonon emission is greater than the quantum well width ‘b/2’, the hole capture rate should be reduced by the probability [1-exp(-b/2l)] that the hole emits optical phonon when crossing the quantum well [18]. The capture time of the hole for the GaN quantum well has been determined by the classical model, which is given by the following relation.

$$\frac{1}{\tau_h} = \frac{2}{b}\sqrt{\frac{\pi m_h^B}{2E_h^B}}\left(1-\exp\left(-\frac{w}{\tau_{h-p}(E_h)v_h^W}\right)\right) \tag{4}$$

where, b/2 is the barrier width, the suffixes B and W are used for barrier and well respectively, w is the well width, τ_{h-p} is the hole scattering time due to optical phonon (h-p) emission. The E_h is the kinetic energy of the hole crossing the quantum well as expressed in equation (5) shows dependence on the laser excess energy E_{excess} , v_h^W

is hole velocity above the quantum well, V_W^h depth of the quantum well in the valence band, m_e and m_h are the electron and heavy hole effective masses in the quantum well regions, respectively [18].

$$E_h = E_{excess}\frac{m_e}{m_e+m_h} + V_W^h \tag{5}$$

$$\Phi = \frac{e^2\omega_L}{2w}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_s}\right) \times \sum_n \frac{\left|\mathrm{F}_{wbe\,(o)}(n)\right|^2}{\sqrt{\left[\left(\frac{n\pi}{w}\right)^2 \frac{\hbar^2}{2m} + E + E_h\right]^2 - 4EE_h}} \tag{6}$$

At this juncture, ε_∞ is the dynamic dielectric constant, ε_s is the static dielectric constant, Φ is the scattering rate of the carrier in the quantum well region which is a function of the quantum well width and energy E with $\mathrm{F}_{wbe(o)}$ for even (odd) wave functions [18] given by the following relations for the scattering rate within the quantum well region.

$$\mathrm{F}_{wbe}(n) = \int_{-w/2}^{w/2} \psi_w(x)\sin\left(\frac{n\pi x}{w}\right)\psi_b(x)dx \tag{7}$$

$$\mathrm{F}_{wbo}(n) = \int_{-w/2}^{w/2} \psi_w(x)\cos\left(\frac{n\pi x}{w}\right)\psi_b(x)dx \tag{8}$$

Here, ψ_w and ψ_b are the general solutions of the Schrödinger equation as given in equation (2). The wave function Ψ_b of the hole in the sub-band is obtained for the different values of Aluminum mole fraction, hole effective mass and the flat Γ band with parabolic energy dispersion, both properly interpolated between GaN and AlN. The transmission coefficient $T_{B\rightarrow W}$ has the form given by equation (9), which permits us to reduce the region of search in the space of parameters for optimization and designing of efficient quantum well laser diode. The transmission coefficient is function of the barrier height, the effective mass of the hole and the kinetic energy E_h:

$$T_{B\rightarrow W} = \frac{4\sqrt{m_h^B m_h\left(E_h - V_w^h\right)E_h}}{\left(\sqrt{m_h^B\left(E_h - V_w^h\right)} + \sqrt{m_h E_h}\right)^2} \tag{9}$$

The energy distribution function for holes in the GaN/AlGaN quantum well laser diode is deduced from the following expressions at 300 K temperature. The Fermi distribution functions shown in equations (10) and (11) have been obtained for the single quantum well structure shown in Fig. 1. The distribution function $f(E)$ [23] given in (10) is for intermediate energies. As the energy increases and reaches $\frac{m_b V}{m_b - m_w}$, the effective well for confined state vanishes. Hence, we had analyzed the energy distribution function for the values of energy E less than $\frac{m_b V}{m_b - m_w}$ in accordance with the expression (11). Here, V is the barrier height of the quantum well structure and in our computation the value of V is greater than E, therefore equation (11) is valid.

$$f(E) = E^{0.5}\left[1.0 - \left\{\frac{m_b}{m_w}\left(1.0 - \frac{V}{E}\right)\right\}^{0.5}\right] * \exp\left(-\frac{E}{k_B T}\right) \tag{10}$$

for $V \le E \le \frac{m_b V}{m_b - m_w}$

$$f(E) = E^{0.5} * \exp\left(-\frac{E}{k_B T}\right) \tag{11}$$

for $E < \frac{m_b V}{m_b - m_w}$

At this juncture the k_B is the Boltzman constant, T is temperature in Kelvin. The effective masses of hole and electron in equations (5) – (11) depend on Aluminum mole fraction x. The relation of effective masses and Aluminum mole fraction x for the $Al_xGa_{1-x}N$ are described as follows:

$$m_e(x) = [0.3x + 0.2(1-x)]m_0 \tag{12a}$$

$$m_h(x) = [3.53x + 1.76(1-x)]m_0 \tag{12b}$$

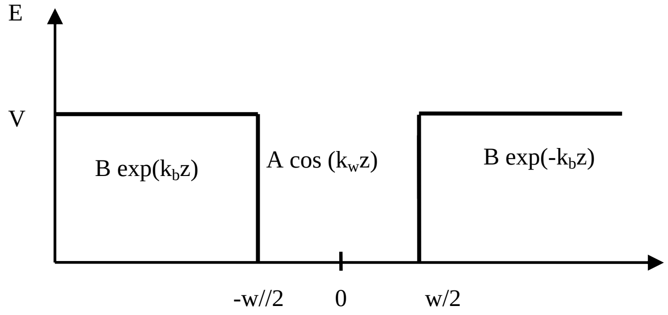

Fig. 1. Single Quantum Well Structure with GaN well and AlGaN barrier.

3. Results and discussion

The carrier capture process is of great significance in the quantum well region. The population inversion occurs due to capturing of electrons and holes in the quantum well region and a short capture time of these carriers reduces the threshold current. Fig. 2 shows the holes capture time dependence on the barrier width and Aluminum mole fraction of AlGaN. The minor variation in hole capture time has been observed due to variations in barrier width and with the increase in barrier width the hole capture time increases linearly as expected. The simultaneous study of the mole fraction dependence has been carried out and Fig. 2 reveals that increase in mole fraction enhances strongly the hole capture time. The hole capture time was found increase from 12 ps to 65 ps for the values of Aluminum mole fraction changing from 0 to 100% respectively. The barrier width was considered to change from 10 nm to 20 nm. The higher capture time is obtained for larger values of the Aluminum mole fraction due to the increase in the band offset between the quantum well and barrier regions.

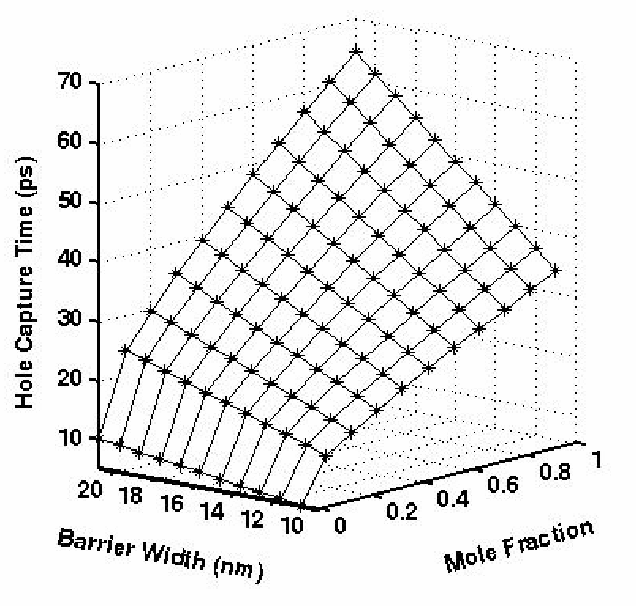

Fig. 2. Hole Capture Time as Function of Barrier Width and Aluminum Mole Fraction in Barrier Region.

The result shown in Fig. 3, ascertains the dependency of the hole capture time on the laser excess energy and the Aluminum mole fraction. It reveals that with the increase in laser excess energy, the hole capture time decreases linearly which consequently infers the improvement in transition of electron from the barrier to the well region. This is mainly due to the increase in kinetic energy of the electrons present in a barrier region, which gains the excess amount of energy and enables them to cross over the barrier region. The large excess energy attributes the broadening and slight shift of the band in short wavelength region. With the increase in Aluminum mole fraction, the effective mass of the AlGaN and the potential depth of quantum well increases, which reduces the transition of the electron from barrier region to the well region and the probability of hole capture decreases and thus resulting greater values of the hole capture time.

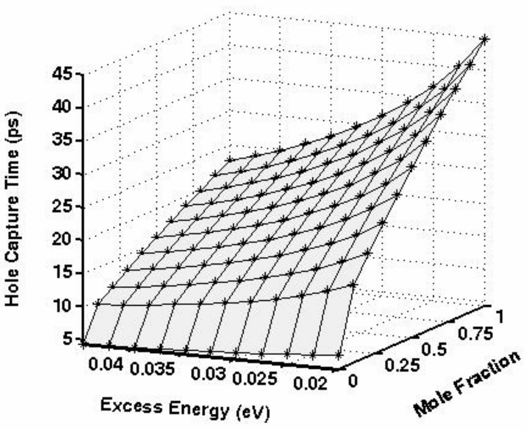

Fig. 3. Dependence of Hole Capture Time on Excess Energy and Aluminum Mole Fraction in Barrier Region.

The transmission coefficient quantifies the proportion of the electrons that tunnel through a barrier. The transmission coefficient is the prospects of an electron intrude on a barrier structure for tunneling which results in contributing the current flow through the barrier. The transmission coefficient obtained through the Schrödinger equation shows its importance in defining the boundary conditions for the Boltzmann equation at the interface between the classical and quantum zones. The mole fraction of the Aluminum in the AlGaN has been increased to enhance the value of the barrier height to observe its influence on the transmission coefficient. The maximum value of transmission coefficient obtained is 0.92 as it is being depicted in Fig. 4. The increase in band offset between the barriers and well causes the decrease in the transmission coefficient and the value of the transmission coefficient is found to be 0.49 for the barrier height of 1.4 eV. It can be explained on the classical basis that it is harder for the electrons to tunnel through higher barrier. The variation in the transmission coefficient is nonlinear with respect to the barrier height while the effect of the barrier width is almost negligible. The transmission losses have not been considered in our analysis and therefore, the transmission coefficient is not showing much variation with the change in barrier width.

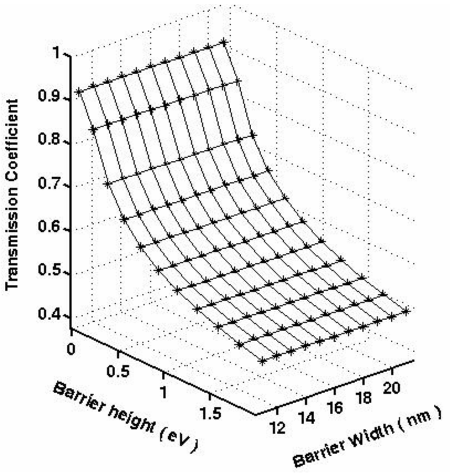

Fig. 4. Variation of Transmission Coefficient with Aluminum Mole Fraction.

The paper covenants to simulate capture events into quantum well structures to understand the carrier phenomena to excavate hole capture times. The study of the hole capture is useful in developing high speed quantum well lasers, for the assurance of fast and efficient hole capture into the quantum confined states to improve the radiative recombination. Therefore, analysis of dependence of hole capture time on quantum well width has been carried out for different mole fractions of Aluminum as shown in Fig. 5. The barrier width was taken 20-nanometer and the effective energy of the holes was deduced to be 0.028 eV. It reveals that with increase in the quantum well width, the hole capture time decreases, while with the increase in Aluminum mole fraction the hole capture time increases. The hole capture time decreases in exponential manner with respect to the quantum well width as it is expected from the relation given in (4). This is due to the reduction of capture rate by the probability that the hole emits optical phonon when crossing the quantum well.

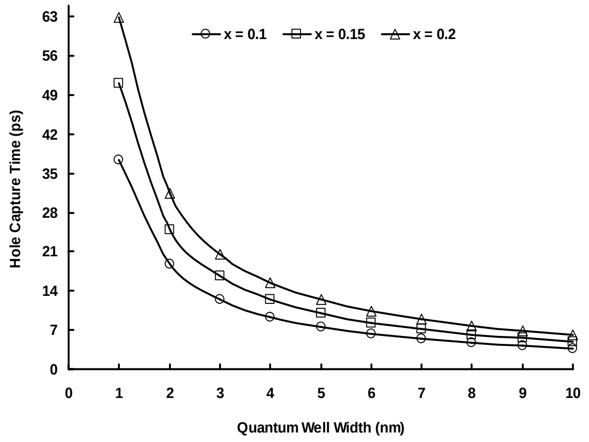

Fig. 5. Hole capture time variation with Quantum Well Width.

The inset of Fig. 6 reveals the scattering rate for a shallow quantum well, while the Fig. 6 shows extended quantum well width up to14 nm to observe the significant effect of the Aluminum fraction on the hole capture time. It reveals that a sudden increase in the hole capture time occurs beyond 8 nm quantum well width. The scattering rate was estimated for the Aluminum mole fraction of 10 %, 15 % and 20%. It is observed that for the higher percentage of Aluminum, the scattering rate reaches to its maximum value for the lower quantum well width. The scattering rate has been deduced from the well-known Fermi Golden rule model and hence the quantum mechanical calculations are predicted to have the resonance. The hole energy is found to be 0.028 eV for 10 % of Aluminum mole fraction and the probability of hole capture by a quantum well and emissions of optical phonon exhibits a number of resonances as function of well thickness as it is expected by Brum and Bastard [24]. The result reveals that for the lower values of Aluminum mole fractions, the scattering rate is showing comparatively lower variations. The high capture time causes more tunneling in the barrier region, which is obvious due to very thin quantum well region [25].

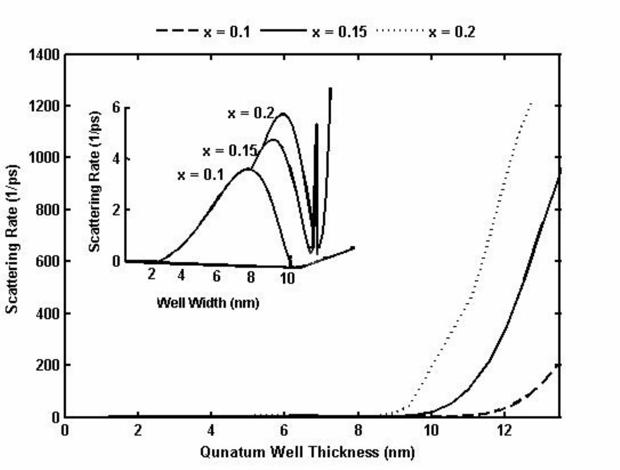

Fig. 6. Scattering Rate of unbound Holes in Single Quantum Well.

The normalized heavy hole energy distribution function for unbound carriers where $m_b > m_w$ has been obtained using equation (11) as shown in Fig. 7. Carrier capture into quantum well is considered by polar optical phonon emission under equilibrium condition. According to quantum mechanical approach, resonances in the capture rate are dependent on the geometry and the material composition of the well. These resonances are attributed to the capture of holes in the unbound states, which have high probability density in the well region. The energy distribution function was found to be changing in non-linear manner as a function of energy. The mass of unbound hole in barrier and well region were considered as 1.856 m_0 and 1.76 m_0 respectively. The mole fraction of Aluminum was taken to be 10 % and distribution has been obtained at lattice temperature of 300 K.

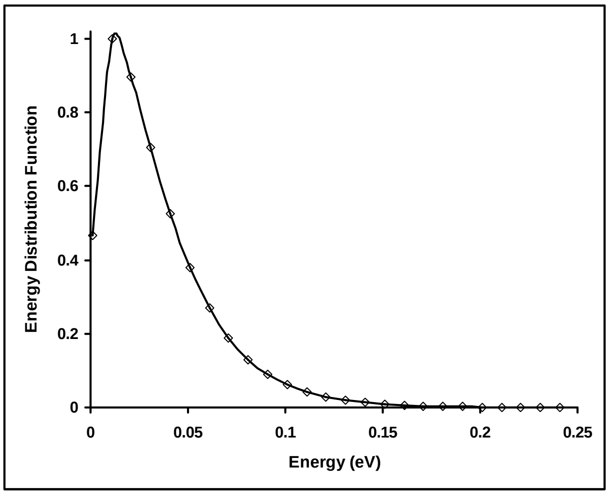

Fig. 7. Normalized Energy Distribution Function for holes.

4. Conclusions

Detail analysis of hole capture in a Gallium Nitride quantum wells has been carried out with hole-optical phonon scattering mechanism using semi-classical model to enhance the performance of quantum well lasers operating with fast switching speeds. The hole capture time was deduced as a function of the excess energy, quantum well width, barrier width and aluminum (Al) mole fraction in the barrier layer. Our analysis reveals strong dependence of hole capture time and scattering rate on the geometry and material composition of the well and the barrier. The hole capture time was found to change from 0.3 ps to 65 ps with variation of structural parameters of the quantum well and Al mole fraction in the barrier. Our analysis provides useful physical insight to improve the performance of the quantum well lasers by proper optimization of structural and material parameters of GaN and AlGaN.

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[*] Corresponding author: patildsp@rediffmail.com