Quantum Physics Letters
An International Journal

http://dx.doi.org/10.18576/qpl/060303

Computer Simulation of Exciton Capture Mechanism in GaN/AlGaN Quantum Heterostructures

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Received: 2 Sep. 2017, Revised: 19 Nov. 2017, Accepted: 23 Nov. 2017

Abstract: Research of the optical properties of III- nitrides quantum well is use to improve the efficiency of optical properties of for light-emitting diodes (LEDs) and laser diodes (LDs) . Also III- nitride semiconductors are used in applications like water sterilization, skin treatment and security.Two dimension multiple quantum well (MQW) & Modified Symmectric Quantum Well (MSQW) carrier confinement are neccessary to increase the efficiency of AlGaN/lGaN .Therefore AlGaN-based materials are suitable for development of ultraviolet light source.Study of optical properties of the specific structure of AlGaN/GaN has been done in this research. Examination of carrier confinement mechanism and the carrier life time by exciting the material in quantum barrier energy under continuous wave operation in the visible spectrum region ranging from green to blue colors is reported in this research. [1] The theoretical analysis for energy band gap, Refractive indices, Dielectric function and model parameters has been carried out and results of simulation along with temperature drift of various parameters are presented. The paper concludes with the possible application of these results in the design of GaN waveguides, which are to be used at the elevated temperatures and for GaN/AlGaN hetero-structure lasers. [2].

Keywords: Exciton, Quantum Heterostructures, Optical Properties, Quantum Well

1 Introduction

Quantum Well (QW) lasers are estimated to show superior lasing properties such as lower threshold current density, higher differential gain as compared to heterostructure laser diodes.The variation of the quantum well width, the thickness of the top barrier layer and the potential depth controls the relations between carriers confined within the well region and surface states. Using MATLAB we have theoroticaly calculated 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. Further the capture time of the electron and the hole in the quantum well shows huge implication in the lasing action and needs the concentration for the expansion of the laser diode efficiency and to lower the threshold current.Emission of optical phonons or carrier-carrier scattering in a layered system.The wide band-gap III?V nitrides has very largr capacity optoelectronic devices emitting in the spectral range from visible to ultraviolet. the refractive indices of GaN and AlGaN and their relative change with temperature is the important part of this research. Another factor is diaelectric function of GaN and AlGaN layers grown under different conditions for a wide spectral range at room temperature by means of spectroscopic ellipsometry. (3)

2 Mathematical Approach

2.1 Phonon Modes and Their Potentials

We use a macroscopic dielectric continuum model to describe the optical phonons in these systems.2 It has been shown, based on lattice dynamical calculations, that the dielectric continuum model gives a good representation of electron-phonon scattering rates in quantum-well systems. Here we use electromagnetic boundary conditions for the phonons that have been shown to give a good representation of electron-phonon scattering rates.5,8 Within each semiconductor material the displacement field satisfies $\nabla\dot{D}$and the electric field is given by $D=\varepsilon(\omega)E$ .The dielectric function is taken to

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be $\varepsilon(\omega) = \varepsilon\infty, n(\omega 2 - \omega 2n, TO)$ where $n = 1$ for GaN $n = 2$for AlGaN, and $\omega n, LO$ $\omega n, TO$ O are the longitudinal- and transverse-optical mode frequencies. Within this approach the frequencies of the confined LO modes are $\omega n, LO$ The interface modes satisfy the condition $\nabla \dot{E} = 0$ that the conditions that E and D' are continuous at the interface sThe parameters used here for GaN are Eg=3.28 ev,me=0.20 mo,mmh =1.4 mo,ε=8.9,mv=1.5mo [4] The quantum-well material is GaN. The barriers and the thin layer in the quantum well are AlGaN All calculations have been done with d=8 . [4] For a simple GaN/AlGaN quantum well of width L, the frequencies of the symmetric interface modes satisfy the condition

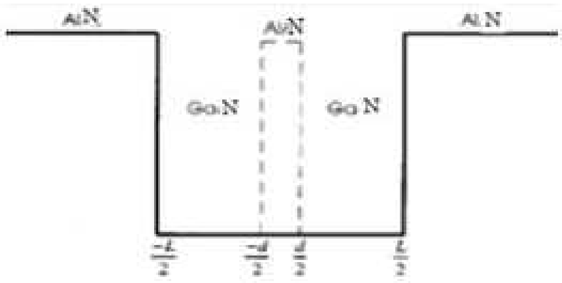

Fig. 1: Sketch of a simple quantum well (SQW)

$$\varepsilon GaN(\omega)\tanh^{(\frac{qL}{2})} = -\varepsilon AlGaN(\omega)...(1)$$

and the antisymmetric modes satisfy

$$\omega GaN(\omega)\coth^{(\frac{qL}{2})} = -\varepsilon AlGaN(\omega)...(2)$$

Applying the same conditions to the quantum well of width L with an additional AlAs layer of width d in the center yields, for the frequencies for the symmetric interface modes of a SMQW,

$$\varepsilon GaN(\omega)\{\varepsilon GaN(\omega)(1+e^{-qd})\tanh^{(}\frac{q(L-d)}{2})$$

$$+$$

$$\varepsilon AlGaN(\omega)\}$$

$$+$$

$$\varepsilon AlGaN(\omega)\{\varepsilon AlGaN(\omega)(1-e^{-qd})\tanh^{(}\frac{q(L-d)}{2})$$

$$+$$

$$\varepsilon GaN(\omega)\}\ldots(3)$$

The antisymmetric interface modes in the SMQW satisfy

$$\varepsilon GaN(\omega)\{\varepsilon GaN(\omega)(1-e^{-qd}$$

$$+$$

$$\varepsilon AlGaN(\omega)\coth^{(}\frac{q(L-d)}{2})\}$$

$$+$$

$$\varepsilon AlGaN(\omega)\{\varepsilon AlGaN(\omega)(1+e^{-qd})$$

$$+$$

$$\varepsilon AlGaN(\omega)\coth^{(}\frac{q(L-d)}{2})\} = 0$$

which gives Semi-classical analysis of hole capture in Gallium Nitride quantum wells In the following we develop a semiclassical model of the heavy hole capture time. Under the collision-free hole transport conditions, the thermionic emission current fills the QW. Then one can estimate the thermionic capture time for a hole using the relation

$$\tau_{therm} = \frac{b}{2}\left(\frac{\pi m_h^B}{2E_h^B}\right)^{\frac{1}{2}} exp\left(\frac{e\Phi}{k_B T}\right)\ldots(3.6)$$

wherem_h^B is the heavy hole effective mass and E_h^B is the hole energy, both in the AlGaN barrier.$e\Phi$ in Eq. (3.6) represents the potential wall for the hole in the AlGaN, created by the space charge. This potential can be estimated from the Poisson equation assuming the spatially independent densities for electrons and holes on the AlGaN barriers. One gets

$$\Phi = \frac{e}{2K^B}(n_e - n_h)\left(\frac{b}{2}\right)^2\ldots(3.7)$$

where K^B is the static permittivity of the AlGaN barrier.Now we wish to argue that in the experiments of interest the barrier $e\Phi$ was negligibly small. Experimental measurements show that there is no dependence of the capture time on an excitation density in the range from 3×10^{15} to $3\times10^{17}cm^{-3}$ These results were obtained for undoped semiconductor QW structures as well as for the semiconductor QW structures with n-doped and p-doped QWs. The absence of density dependence of the carrier capture time in such a broad range of carrier densities strongly suggests that $\frac{e\Phi}{k_BT} \approx 1$We can then estimate from that the space charge density in the AlGaN barrier, $n_e - n_h$,is smaller than $2.5\times10^14cm^{-3}$ Certain number of holes remains in the barrier because they are electrostatically repulsed by holes captured in the QW. In the same time, the electron density decreases owing to the electron attraction by the holes captured in the QW. As a consequence of this ambipolar process, the electron and hole densities in the barrier tend to remain the same. Thus Eq. (3.6) can be reduced to a simple relation, [3]

$$\tau_{therm} = \frac{b}{2}\left(\frac{\pi m_h^B}{2E_h^B}\right)^{\frac{1}{2}}\ldots(3.8)$$

If the hole mean free path due to the polar optical phonon emission, ℓ is greater than the GaN QW width w, the hole capture rate should be reduced by the probability $\{1 - exp(-w/\ell)\}$ that the hole emits optical phonon when crossing the QW:

$$\frac{1}{\tau} = \frac{1}{\tau_{therm}} \left(1 - e^{-\frac{w}{\ell}}\right) \ldots (3.9)$$

If we assume that the hole is moving in the barrier as a classical particle, then the phonon emission probability in the QW is

$$1 - e^{-\frac{w}{\ell}} = 1 - exp\left(-\frac{w}{\tau_{h-p}(E_h) v_h^W}\right) \ldots (3.10)$$

where v_h^W is the z-component of the hole velocity above the QW.The hole scattering time due to the optical phonon (h-p) emission reads

$$\frac{1}{\tau_{h-p}(E_h)} = \frac{1}{\tau_{h-pop}(E_h)} + \frac{1}{\tau_{h-nop}(E_h)} \ldots (3.11)$$

$$E_h = E_{excess} \frac{m_e}{m_e + m_h} + V_w^h \ldots (3.12)$$

is the kinetic energy of the hole crossing the QW, Excess is the laser excess energy,V_w^h is the depth of the QW in the valence band, and me and mh are the electron and heavy hole effective masses in the QW, respectively.The first term on the right-hand side of Eq. (3.11) is the emission rate via the heavy hole-polar optical phonon (h-pop) interaction which has the form

$$\frac{1}{\tau_{h-pop}(E_h)} = \sqrt{\frac{m_k}{2}} \frac{e^2 \omega LO}{4\pi h} \left(\frac{1}{K_\infty} - \frac{1}{K}\right) \frac{1}{\sqrt{E_h}} ln$$

$$\left| \frac{\sqrt{E_h} + \sqrt{E_h - \hbar\omega LO}}{\sqrt{E_h} - \sqrt{E_h - \hbar\omega LO}} \right| \ldots (3.13)$$

Where ωLO is the frequency of longitudinal optical phonons K and K_∞ are the static and high frequency permittivities, respectively, in the QW. The second term represents the heavy hole non polar optical phonon (h-nop) emission rate in the form

$$\frac{1}{\tau_{h-nop}(E_h)} = \frac{(2mh)^{3/2} D^2 0}{4\pi \hbar^3 \rho \omega_0} \sqrt{E_h - \hbar\omega_0} ..(3.14)$$

where $D0$ is the non polar optic deformation potential,ρ is the mass density vL is the velocity of sound, and ω_0 is the non polar optic phonon frequency In Eq. (3.10) the z-component of the hole velocity can be found from the laser excess energy as

$$V_h^W = \sqrt{\frac{2}{m_h} \left(\frac{1}{3} E_{excess} \frac{m_e}{m_e + m_h} + V_w^h\right)} ..(3.15)$$

The model (3.8)-(3.10) can be further improved if we take into account that the carrier can be quantum-mechanically reflected at the edges of the QW (at points $-w/2$ and $w/2$).Then

$$\frac{1}{\tau} = \frac{2}{b} \left[\frac{2E_{excess}}{3\pi (m_e^B + m_h^B)} \frac{m_e^B}{m_h^B} \right]^{1/2}$$

$$T_B \rightarrow W \left[1 - exp\left(- \frac{w}{\tau_{h-p}(E_h) v_h^W T_W \rightarrow B} \right) \right] ..(3.16)$$

and m_e^B e is the electron effective mass in the 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.

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 [3].

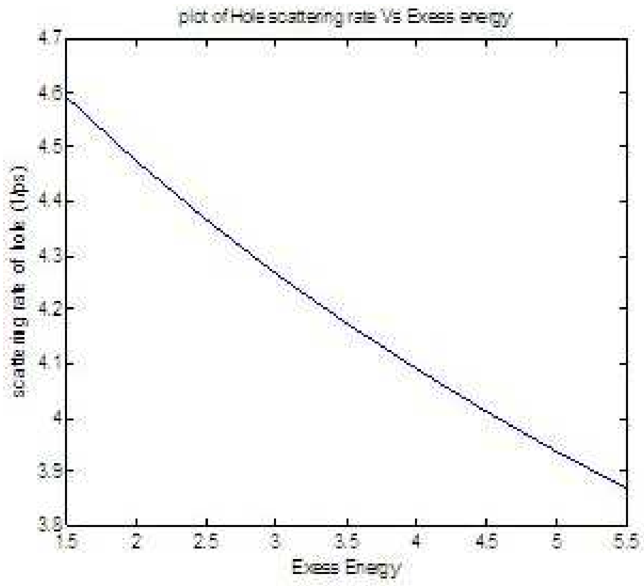

Fig. 2: Variation of Scattering Rate of hole With Excesses Energy of hole

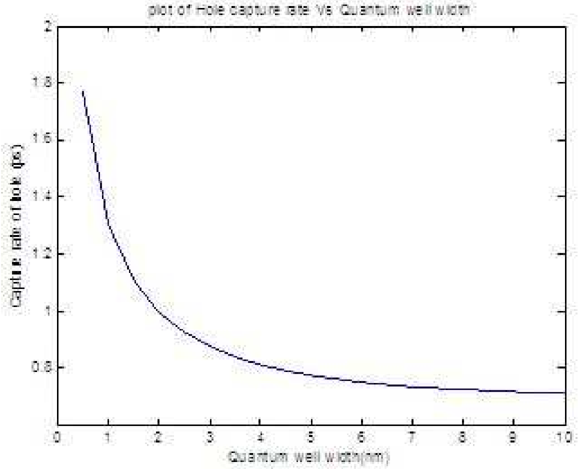

Fig. 3: Variation of capture rate of hole(ps) with Quantum well width(nm)

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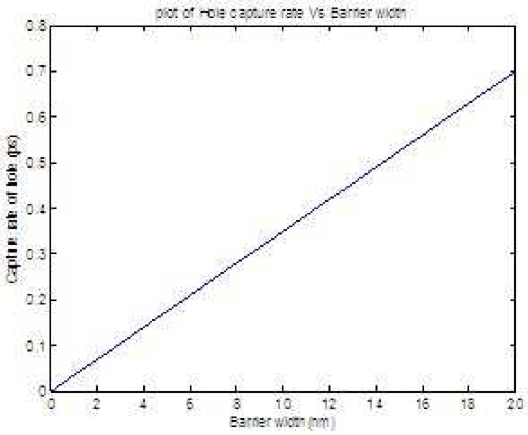

Fig. 4: Variation of capture rate of hole(ps) with Barrier width(nm)

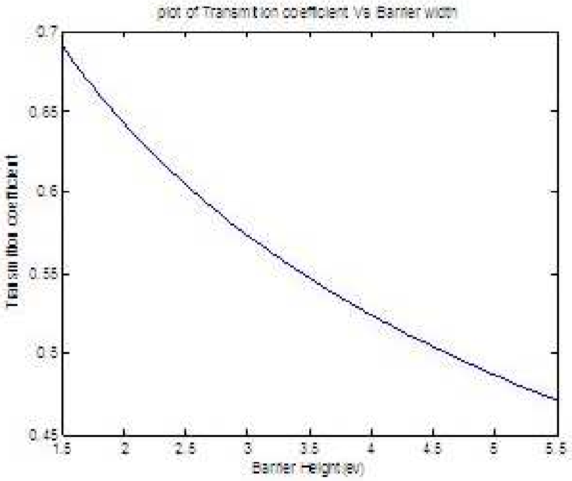

Fig. 5: Variation of Transmission Coefficient with Barrier height.

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