



# Pressure induced interband emission energy in a nitride based wide band gap quantum dot

N.S.Minimala<sup>1</sup> and A.John Peter<sup>2\*</sup>

<sup>1</sup>Department of Physics, N.M.S.Sermathai Vasan College for Women, Madurai-625 012.

<sup>2</sup>Department of Physics, Government Arts College, Melur-625 109, Madurai.

## ARTICLE INFO

### Article history:

Received: 1 August 2012;

Received in revised form:

31 August 2012;

Accepted: 20 September 2012;

### Keywords

Pressure,  
Band gap,  
Quantum,  
Interband.

## ABSTRACT

Effect of pressure on the ground state exciton binding energy and the interband emission energy in a wurtzite GaN quantum dot are investigated. The interband emission energy is computed as a function of pressure with a constant geometrical confinement. All the numerical calculations are performed using variational procedure within the single band effective mass approximation. The internal electric fields comprise the spontaneous polarization and piezo electric polarization are included in the Hamiltonian. Our results show that the effects of pressure and the geometrical confinement have great influence on the optical properties of this wide band gap nitride based group-III quantum dots.

© 2012 Elixir All rights reserved.

## Introduction

Group-III nitride materials show interesting behaviour in opto-electronic devices such as Light emitting diodes and Laser diodes [1]. The recent progress in group-III nitride based low dimensional semiconductor systems shows the importance of built-in electric fields due to both spontaneous polarization and piezoelectric effects. A linear variation of internal fields is observed upto the Al alloy content, 0.27 [2].

### Model and theory

An exciton confined in a GaN quantum dot with a spherical potential barrier (AlGaIn) with the confining potential is considered and it is assumed to be zero inside and V outside. The conduction and valence bands are centered around the  $\Gamma$  valley of GaN and AlGaIn. The Schrödinger for the exciton is then given by

$$H_{exc} \psi(r_e, r_h) = E_{exc} \psi(r_e, r_h) \quad (1)$$

Within the framework of single band effective mass approximation, the Hamiltonian of a strained GaN / AlGaIn quantum dot with the radius R, in the presence of pressure, incorporating the effect of piezoelectric field, is written as,

$$H_{exc}(P) = -\frac{\hbar^2}{2m_e^*(P)} \nabla_e^2 + V_e(\bar{r}_e, P) - \frac{\hbar^2}{2m_h^*(P)} \nabla_h^2 + V_h(\bar{r}_h, P) - \frac{e^2}{\epsilon(P)|\bar{r}_e - \bar{r}_h|} + \pm |e| F(P)z \quad (2)$$

where  $m_{e(h)}^*(P)$  is the pressure dependent effective mass of electron (hole),  $e$  is the absolute value of electron charge,  $V_{e(h)}(r_{e(h)}, P)$  represent the pressure dependent confinement potential for the electron (hole) respectively,  $F(P)$  is the pressure dependent effective electric field due to piezoelectric effect,  $\epsilon(P)$  is the pressure dependent dielectric constant of the material inside the quantum dot,  $|\bar{r}_e - \bar{r}_h|$  denotes the relative distance between the electron and the hole.

The ground state wave function of the electron (hole) confined in the strained GaN / AlGaIn quantum dot can be written as

$$\psi(r_j) = \frac{1}{r_j} \varphi(r_j) Y_l^m(\theta, \phi) \quad (3)$$

Where  $Y_l^m(\theta, \phi)$  are the complex spherical harmonics and  $\varphi(r)$  is the radial wave function and the corresponding confinement energy equation of the electron (hole) can be obtained by using the  $m$ -order Bessel function  $J_m$  and the modified Bessel function  $K_m$  as

$$\psi(r, \theta, \phi) = \begin{cases} N_1 J_l(r_{nl} r) e^{-\alpha r} e^{\pm i l \phi} & r < R \\ N_1 \frac{J_l(r_{nl} R)}{K_l(b_{nl} R)} e^{-\alpha r} e^{\pm i l \phi} K_l(b_{nl} r) & r \geq R \end{cases} \quad (4)$$

where  $\alpha$  is the variational parameter and  $N_1$  the normalization constant. The interband emission energy  $E_{ph}$  associated with the exciton is calculated using the following equation

$$E_{ph}(P) = E_e + E_h + E_g^\Gamma - E_{exc}(P) \quad (5)$$

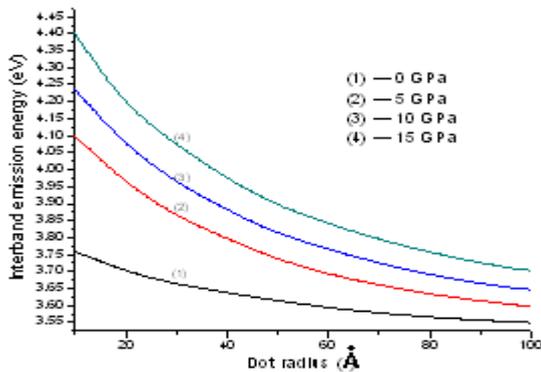
where  $E_e$  and  $E_h$  are the confinement energies of the electron and hole respectively.

### Results and discussion

The carried out calculations are done on computing the exciton binding energy and thereby the interband emission energy in the influence of hydrostatic pressure and the effects of geometrical confinement in the spherical GaN / AlGaIn quantum dot. Heavy hole has been taken for all our calculations since the heavy hole mass as the heavy excitons are more common in experimental results. The atomic units have been followed in the determination of electronic charges and wave functions in which

the electronic charge and the Planck's constant have been assumed as unity.

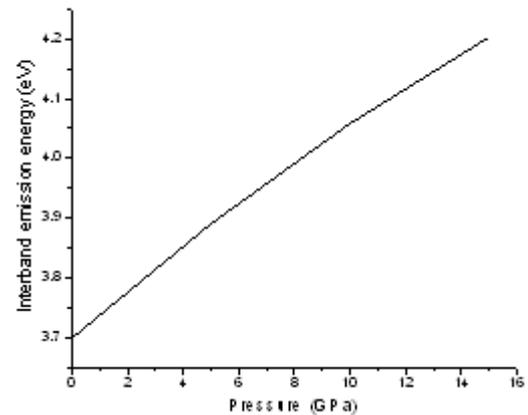
We present the variation of interband emission energy as a function of dot radius in the presence of pressure in a GaN/Al<sub>x</sub>Ga<sub>1-x</sub>N quantum dot for  $x = 0.2$  in Fig.1. It is observed that the interband emission energy decreases monotonically as the radius of dot is increased for all the pressure. This is due to the confinement of electron-hole with respect to z-plane when the dot radius is increased. This representation clearly brings out the quantum size effect. Moreover, it is observed that interband emission energy increases with the pressure. It is because the exciton binding energy increases with the pressure. Moreover, we notice that the effective of interband emission energy is more pronounced for smaller dot sizes irrespective of application of pressure. The electron-hole confinement is increased when the pressure effect is included in the Hamiltonian.



**Fig.1 Variation of interband emission energy as a function of dot radius in the presence of pressure, for  $x = 0.2$ , in a GaN/Al<sub>x</sub>Ga<sub>1-x</sub>N quantum dot.**

Fig.2 displays the variation of interband emission energy as a function of pressure with a constant  $x = 0.2$ , in for a 20Å GaN/Al<sub>x</sub>Ga<sub>1-x</sub>N quantum dot. It is observed that the interband emission increases with the pressure linearly [2] due to the confinement. This increase in exciton binding energy with the

applied hydrostatic pressure reflects the additional confinement due to the external pressure and the changes in effective mass and dielectric constant. We hope that the present results would motivate some experimental research on group-III nitride materials to improve the fabrications on optical devices.



**Fig.2 Variation of interband emission energy as a function of pressure with a constant  $x = 0.2$ , in for a 20Å GaN/Al<sub>x</sub>Ga<sub>1-x</sub>N quantum dot**

### Conclusion

The optical properties of an exciton confined in a GaN/Al<sub>x</sub>Ga<sub>1-x</sub>N quantum dot have been studied in the presence of hydrostatic pressure assuming a spherical confinement potential. The effects of strain and the internal field due to spontaneous and piezo-electric polarizations have been included in all our calculations. It has been brought out that the geometrical confinement and the application of pressure will alter the optical properties.

### Reference

- 1.H.Sihau and B.Shiliang, J. Semiconductors, 29 (2008) 234.
2. P. Bigenwald, P. Lefebvre, T. Bretagnon and B. Gil , phys. stat. sol. (b) 216 (1999) 371.