Electric Field Effects on the Confinement Properties of GaN/Al$_x$Ga$_{1-x}$N Zincblende and Wurtzite Nonabrupt Quantum Wells

H. Wang, G. A. Farias, and V. N. Freire
Departamento de Física, Universidade Federal do Ceará,
Caixa Postal 6030, Campus do Pici, Centro de Ciências,
60455-760 Fortaleza, Ceará, Brazil

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We investigate the confinement properties of GaN/Al$_x$Ga$_{1-x}$N zincblende and wurtzite nonabrupt quantum wells (QWs) in an electric field. It is shown that their Stark shifts decrease considerably when the existence of nonabrupt interfaces are considered. Confined excitons in 50 Å wide GaN/Al$_{0.3}$Ga$_{0.7}$N zincblende and wurtzite quantum wells (QWs) can exist up to electric field intensities of the order of 500 kV/cm. In all cases, the electric field effects in GaN/Al$_x$Ga$_{1-x}$N wurtzite QWs are stronger than in similar zincblende QWs.

I Introduction

Visible and ultraviolet emission properties of GaN, AlN and InN based quantum wells (QWs) are continuously finding technological applications in light-emitting diodes and lasers. [1, 2, 3, 4] Nevertheless, their optical emission mechanisms are still a matter of controversy. [5] Localized and trap states related to compositional fluctuations and defects seem to be relevant for the understanding of nitride QWs optical properties, [6, 7, 8] but confined excitons continue to be a key mechanism to explain gain, absorption, and photoluminescense spectra. [9] However, detailed works concerning excitons in GaN/Al$_x$Ga$_{1-x}$N QW structures were published only recently [10, 11, 12] since a better knowledge of the fundamental parameters (gap energy, carriers effective mass, band offset) of nitride semiconductors became possible only after a wealth of experiments and first principle calculations.

Using a variational technique in momentum space and within the effective mass approximation, Chung and Chang [10] have calculated the effects of well width and Al molar fraction in the barrier region on the exciton peak and binding energy in wurtzite GaN/Al$_x$Ga$_{1-x}$N QWs. Although the exciton binding energy they calculated is about 10 meV lower than the bulk GaN exciton energy, Chung and Chang [10] have obtained a good agreement with available experimental data for well widths shorter than 100 Å. Bigenwald *et al* [11] performed a careful study of the electronic and optical properties of wurtzite GaN/Al$_x$Ga$_{1-x}$N QWs in the context of a six-band envelope function approach, obtaining a large well limit behavior for the exciton binding energy similar to that of Chung and Chang, [10] but a higher exciton binding energy for shorter well widths. Wang, Farias, and Freire [12] have studied the role of non-abrupt interfaces on the exciton energy in zincblende and wurtzite GaN/Al$_x$Ga$_{1-x}$N QWs within the effective mass approximation. By using a simple parabolic band scheme, they were successful in obtaining an asymptotic behavior for the exciton binding energy compatible with those of the bulk zincblende and wurtzite GaN exciton energy. Wang, Farias, and Freire [12] showed that the exciton energy in zincblende GaN/Al$_x$Ga$_{1-x}$N QWs is a little higher than in similar wurtzite QWs, and that the existence of non-abrupt interfaces can strongly blueshift the exciton energy depending on the well and interfaces width.

Despite the technological difficulties to have good electric contacts in the nitride semiconductor samples, [13] future transistors and photodetectors based on them should take advantage of their optoelectronic properties. To the knowledge of the authors, no investigation seems to have been performed on the properties of excitons in zincblende and wurtzite GaN/AlN QWs subjected to an electric field, which is addressed in this work for the first time. The existence of nonabrupt interfaces is considered, and the calculations are performed within the effective mass approximation. It is shown that GaN/Al$_x$Ga$_{1-x}$N zincblende and wurtzite QW excitons can continue to exist up to electric intensities of the order of 500 kV/cm. Nonabrupt interfaces can enhance considerably the Stark shifts, which are stronger in zincblende than in wurtzite GaN/Al$_x$Ga$_{1-x}$N QWs.

II Model description and equations

Although GaN/Al$_x$Ga$_{1-x}$N QWs in the wurtzite phase continue to be the most common due the advantage of sapphire substrates in the growth process, there is increasing interest in zincblende GaN/Al$_x$Ga$_{1-x}$N QWs to take advantage of the higher GaN zincblende saturated electron drift velocity and lower band energy for technological applications. [14] The description of wurtzite and zincblende nonabrupt QW interfaces can be performed based on the assumption the Al$_x$Ga$_{1-x}$N energy gap and carrier effective mass dependence on x in both the phases is valid for very thin layers. The interface region begins/finishs at the border of the otherwise abrupt QWs, and can be described after an adaptation of the approach of Freire, Auto, and Farias [15] used to study the role of interfaces in GaAs/Al$_x$Ga$_{1-x}$As. Accordingly, the Hamiltonian describing the electron and hole confinement in both wurtzite and zincblende GaN/Al$_x$Ga$_{1-x}$N nonabrupt QWs subjected to an electric field F is given by:

$$H = E_g^{GaN} - \frac{\hbar^2}{2\mu}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right] - \frac{e^2}{\epsilon\,[\rho^2 + (z_e - z_h)^2]^{1/2}}$$
$$- \frac{\hbar^2}{2}\frac{\partial}{\partial z_e}\frac{1}{m_e^{\perp}(z_e)}\frac{\partial}{\partial z_e} + V_e(z_e) - eFz_e - \frac{\hbar^2}{2}\frac{\partial}{\partial z_h}\frac{1}{m_h^{\perp}(z_h)}\frac{\partial}{\partial z_h} + V_h(z_h) + eFz_h \quad , \qquad (1)$$

where ρ, ϕ, z_e and z_h are the relative electron-hole cylindrical system coordinates; E_g^{GaN} is the GaN gap energy; ϵ is the dielectric constant in the GaN QWs (here $\epsilon = 9.5$ are set for both wurtzite and zincblende structures); μ is the reduced mass corresponding to the electron-heavy-hole pair which is defined as $\mu \equiv m_e^{\parallel} m_h^{\parallel}/(m_e^{\parallel} + m_h^{\parallel})$ ($m_e^{\parallel}$ and $m_h^{\parallel}$ are the effective masses of electron and heavy-hole, respectively, in the plane of the layers); $m_\alpha^{\perp}(z)$ and $V_\alpha(z_\alpha)$ is, respectively, the α-type carrier effective mass and the nonabrupt confinement potential along the growth direction z, which are given by the following expressions:

$$m_\alpha^{\perp}(z_\alpha)/m_0 = m_{\alpha,GaN}^{\perp}/m_0 + (m_{\alpha,AlN}^{\perp}/m_0 - m_{\alpha,GaN}^{\perp}/m_0)\, y(z_\alpha) \quad , \qquad (2)$$

$$V_\alpha(z_\alpha) = \begin{cases} Q_\alpha\ [\ 1.78\, y(z_\alpha) + y^2(z_\alpha)]\quad (eV)\ , & \text{for wurtzite} \\ Q_\alpha\ [\ 2.17\, y(z_\alpha) + 0.53\, y^2(z_\alpha)]\quad (eV)\ , & \text{for zinc-blende} \end{cases} \qquad (3)$$

where Q_α is the band offset for the $\alpha-$type carrier (here, $Q_e/Q_h = 0.7/0.3$ for both wurtzite and zincblende structures); $y(z_\alpha) = x\{1 - \frac{1}{2}[erf(\frac{w-l+2z_\alpha}{l/2}) + erf(\frac{w-l-2z_\alpha}{l/2})]\}$; w and l is, respectively, the well and the interface width; m_0 is the free space electron mass.

Since an analytical solution of the Schrödinger equation for the Hamiltonian describing the nonabrupt GaN/Al$_x$Ga$_{1-x}$N single QWs [see Eq. (1)] is not possible, a variational approach solution is resorted. By disregarding the electron-heavy-hole interaction, numerical solutions $\Psi_e(z)$ and $\Psi_h(z)$ are obtained for the independent electron and hole confinement through the multistep method of Ando and Itoh. [16] Restricting to the ground state, the exciton binding energy is calculated within a variational approach through a minimization process as described by:

Table 1 - Some fundamental parameters of GaN and AlN in the zincblende and wurtzite phases.

Sample	E_g (eV)	$m_e^{\perp}/m_0$	$m_h^{\perp}/m_0$	$m_e^{\parallel}/m_0$	$m_h^{\parallel}/m_0$
GaN (zincblende)	3.3 $^{(17)}$	0.19 $^{(18)}$	0.86 $^{(18)}$	0.19 $^{(18)}$	2.00 $^{(18)}$
AlN (zincblende)	6.0 $^{(19)}$	0.33 $^{(18)}$	1.43 $^{(18}$	0.33 $^{(18)}$	4.55 $^{(18)}$
GaN (wurtzite)	3.5 $^{(20,21)}$	0.19 $^{(18)}$	2.00 $^{(18)}$	0.23 $^{(18)}$	2.04 $^{(18)}$
AlN (wurtzite)	6.28 $^{(22)}$	0.35 $^{(18)}$	3.53 $^{(18)}$	0.35 $^{(18)}$	11.14 $^{(18)}$

$$E_B = -\min_{\lambda}\langle\Psi(z_e, z_h, \rho)|H|\Psi(z_e, z_h, \rho)\rangle \quad . \tag{4}$$

where the trial wavefunction is $\Psi(z_e, z_h, \rho) = \psi_e(z_e)\psi_h(z_h)\psi_{e-h}(\rho)$, with $\psi_{e-h}(\rho) = \left(\frac{2}{\pi\lambda^2}\right)^{1/2}\exp(-\rho/\lambda)$. The ground state exciton energy as a function of the well and interface widths is given by:

$$E_{ex}(w,l) = E_{g,GaN} + E_e(w,l) + E_h(w,l) - E_B(w,l) \quad , \tag{5}$$

where $E_e(w,l)$ and $E_h(w,l)$ is, respectively, the electron and heavy-hole ground state energy in the nonabrupt zincblende and wurtzite GaN/Al$_x$Ga$_{1-x}$N QWs. Table 1 presents the parameters values used during the numerical calculations, which are a survey of data from refs. (17-22).

III Results and discussions

The ground state confinement properties of electron (e) and heavy-holes (hh) in 50 Å wide zincblende and wurtzite nonabrupt GaN/Al$_{0.3}$Ga$_{0.7}$N QWs was calculated. It was obtained that, independent of the interface width, the carriers can remain bound in their ground states up to electric field intensities of the order of 500 kV/cm, allowing the existence of ground state confined excitons since the bulk GaN ground state exciton energy in both the phases is of the order of 28 meV. [23] This behavior can be observed in Fig. 1, where it is depicted the e-hh exciton binding energy in both the zincblende (top) and wurtzite (bottom) GaN/Al$_{0.3}$Ga$_{0.7}$N QWs as a function of the applied electric field for interface widths $l = 0$ Å (abrupt case, dashed), $l = 10$ Å (solid) and $l = 15$ Å (dotted).

One can observe in Fig. 1 that, for a given electric field intensity, the exciton binding energy is always a little higher in the GaN/Al$_{0.3}$Ga$_{0.7}$N wurtzite QW than in a similar zincblende QW. This is due to the values of the parameters related to the band structure of both the phases (see Table 1). As a consequence of the Stark effect, the exciton binding energy decreases when the electric field becomes stronger. Since the ground state Stark shift (which is negative) decreases considerably when the existence of nonabrupt interfaces are considered, the variation of the exciton binding energy with the electric field is smaller for wider interfaces.

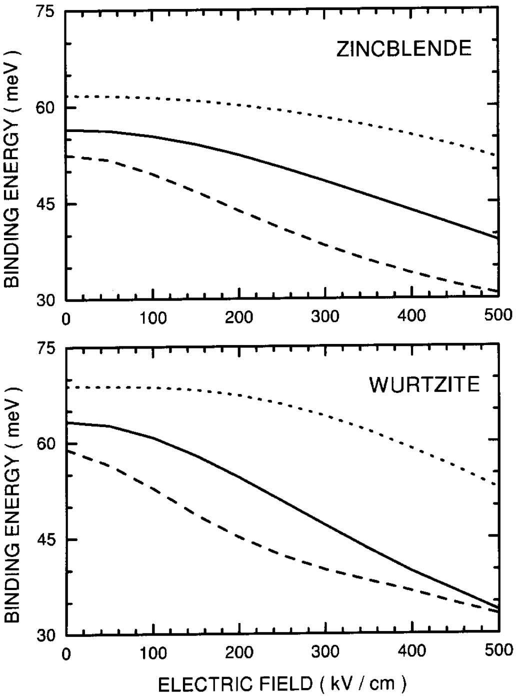

Figure 1. The binding energy $E_B(w,l)$ of excitons in 50 Å wide zincblende (top) and wurtzite (bottom) nonabrupt GaN/Al$_{0.3}$Ga$_{0.7}$N QWs subjected to electric fields, and with sharp (dashed), 10 Å (solid), and 15 Å (dotted) interfaces.

Fig. 2 presents the dependence of the exciton energy on the electric field intensity and on the quantum well interface width. The exciton energy is shown to decrease when the electric field is stronger. The rate of decreasing is considerably modified as a consequence of the nonabrupt interface related blue shift of the carriers energy. As a matter of fact, the exciton energy variation produced by a 500 kV/cm electric field in the zincblende (wurtzite) QW is 53 meV (66 meV) if their interfaces are sharp, while it is only 27 meV (25 meV) if the QW interfaces are 10 Å wide. One can also observe in Fig. 2 that the interface related blue shift of the confined exciton energy in the QWs is stronger when the electric field intensity increases.

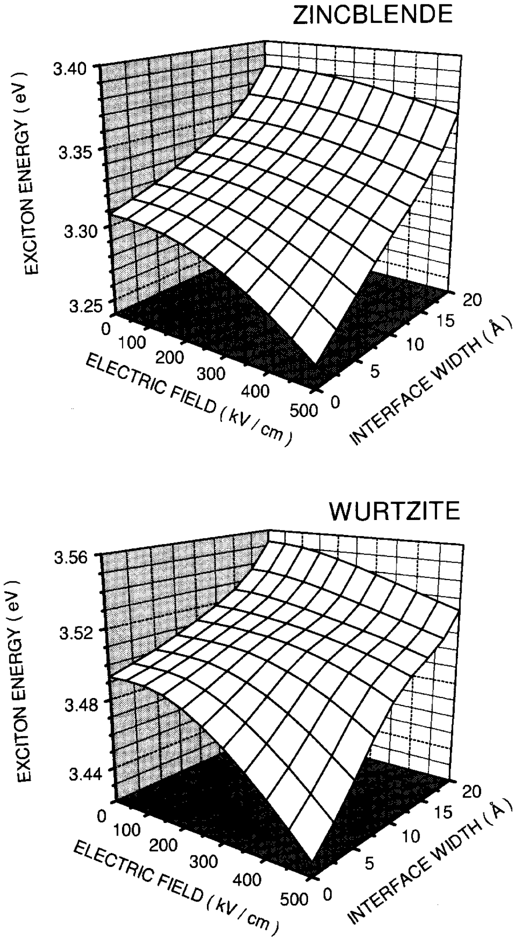

Figure 2. The confinement exciton energy $E_{ex}(w,l)$ in 50 Å wide zincblende (top) and wurtzite (bottom) nonabrupt GaN/Al$_{0.3}$Ga$_{0.7}$N QWs.

IV Concluding Remarks

Although results on the heterointerface characterization of III-V nitride semiconductor quantum wells are sparse, it is possible to estimate that their interface width should be at least of the order of the GaAs/Al$_x$Ga$_{1-x}$As QWs (which is about two GaAs unit cells, *i.e.* $\sim$ 11 Å). Recently, a blue shift in the photoluminescense spectra was associated to QW thickness fluctuations, [24] while phonon mode broadening in GaN/AlN superlattices was related to the existence of graded interfaces [25], indicating that nonabrupt interfaces should be responsible for important changes on the optical properties of actual GaN/Al$_x$Ga$_{1-x}$N QW structures. The results presented in this work have highlighted that interface effects in single GaN/Al$_x$Ga$_{1-x}$N QWs can be more relevant than in similar GaAs/Al$_x$Ga$_{1-x}$As QWs. They suggest that to a better description of the confinement exciton related optical properties, it is necessary to resort a nonabrupt description of the GaN/Al$_x$Ga$_{1-x}$N QWs. The results presented in this work are worth of experimental confirmation.

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