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Exciton Confinement in InGaN/GaN Cylindrical Quantum Wires

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We investigate the confined exciton properties in InGaN/GaN cylindrical quantum wires. We have solved numerically Schrödinger-like equations in the effective mass approximation and have found the energy levels and wavefunctions for confined electrons and holes, using these results to calculate variationally the confined exciton energy. A comparison was made between graded and abrupt quantum wires, showing that the existence of smooth interfaces enhances the confined exciton energy if the wire radius is smaller than 50 Å. We conclude that the existence of graded interfaces must be considered for a better description of the exciton based optical properties of InGaN/GaN quantum wires.

1 Introduction

Blue and ultraviolet light emitting diodes (LEDs) and blue laser diodes (LDs) have been developed recently using In-GaN quantum wells (QWs) as the active layers [1,2]. However, by comparing the density of states of 3D, 2D, and 1D systems, it is clear that a device operating in one dimension has potential to be more efficient than 3D and 2D dimensional devices. This has motivated extensive research in nanowire technology, including the aim of understanding fundamental 1D physics and material proceses.

Recently, Han *et al.* [3] reported the fabrication of GaN nanorods, while Li *et al.* [4] have grown nanoporous GaN structures from crystalline GaN on conducting SiC substrate using etching in HF/H$_2$O$_2$. These structures have shown a blueshifted emission correlated with the development of highly anisotropic wire-like structures in the morphology, with the higher energy cathodoluminescence band arising from the portion of the structure with the smallest feature sizes. Krost *et al.* [5] have found pure metallic indium in thick (300 nm) MOCVD-grown InGaN layers incorporated in a wire-like manner along the growth direction. Such indium wires could act as highly conducting channels harmful for electronic and optoelectronic applications.

We investigate the ground state confined exciton properties. In cylindrical wurtzite In$_{0.2}$Ga$_{0.8}$N/GaN quantum wires. Since interfaces 1-1.5 nm thick in Al-GaN/InGaN/GaN heterostructures were demonstrated [6,7] we take into account their existence.

2 The numerical method

The In$_{0.2}$Ga$_{0.8}$N/GaN cylindrical quantum wires are modeled as follows. The InN molar fraction depends on the distance from the wire axis according to:

$$\chi(r) = 0.1 \left\{ 1 - \mathrm{erf}\left(\frac{2(r-R) + \sigma}{\sigma/2} \right) \right\},$$

where R is the quantum wire radius and σ is the graded interface thickness. The effective mass approximation is adopted, and the BenDaniel-Duke kinetic energy operator is part of the exciton Hamiltonian:

$$\widehat{H} = E_g(\chi = 0.2) \underbrace{- \frac{\hbar^2}{2}\nabla_e \left(\frac{1}{m_e(r_e)} \right) \nabla_e + V_e(r_e)}_{\widehat{H}_e}$$

$$\underbrace{- \frac{\hbar^2}{2}\nabla_h \left(\frac{1}{m_h(r_h)} \right) \nabla_h + V_h(r_h)}_{\widehat{H}_h} \underbrace{- \frac{e^2}{4\pi\varepsilon\varepsilon_0 |\mathbf{r_e} - \mathbf{r_h}|}}_{\widehat{V}_{eh}},$$

where $m_e(m_h)$ and $V_e(V_h)$ are, respectively, the electron (heavy hole) effective mass and confinement potential. The effective masses are isotropic, calculated by averaging in the parallel and perpendicular directions to the [0001] growth axis; ε is the In$_{0.2}$Ga$_{0.8}$N dielectric constant. The confinement potentials, on the other hand, depend on the band offsets, taken here to be $Q_e = 0.7$, $Q_h = 1 - Q_{e=}0.3$; the bowing parameter is assumed to be b=2.6 eV [8]. The parameters for the In$_{0.2}$Ga$_{0.8}$N alloy were obtained by interpolation of the InN and GaN presented in Table I.

The variational wavefunction we used for the exciton ground state is:

$$\psi_{eh} = \psi_e(r_e)\psi_h(r_h) e^{-\frac{\sqrt{r_e^2 + r_h^2 - 2\beta r_e r_h}}{\lambda}} e^{-\frac{z_e^2 + z_h^2}{\lambda}},$$

Table I - InN and GaN data [8,9].

	InN	GaN
E_g **(eV)**	2.050	3.520
m_e/m_o	0.125	0.206
m_h/m_o	1.547	1.081
ε	14.60	10.30

where $z_i (i = e, h)$ is the carrier coordinate measured along the quantum wire axis, which is the growth direction [0001]; ψ_i is the ground state solution of $H_i\psi_i = E_i\psi_i$. λ and β are two variational parameters associated to the radius and symmetry of the ground state exciton, respectively. The exciton grounde state energy is obtained variationally through the following expression:

$$E_{EXC}^0 = \min_{\lambda,\beta} \frac{\langle \psi_{eh}| \widehat{\mathrm{H}} |\psi_{eh}\rangle}{\langle \psi_{eh} \mid \psi_{eh}\rangle},$$

where $E_B^0 = E_{EXC}^0 - E_g(\chi = 0.2) - E_e - E_h$ is the exciton binding energy.

3   The confined exciton

Figure 1 shows the binding (top) and total exciton (bottom) energies in graded $In_{0.2}Ga_{0.8}N/GaN$ cylindrical quantum wires for interface thicknesses ranging from 0 (abrupt quantum wire) to 15 Å. The exciton binding energy in the case of an abrupt wire varies from 55 meV (R=20 Å) to 24 meV (R=80 Å). When a graded interface 10 Å (15 Å) is considered, the binding energy increases by as much as 8 meV (10 meV) when R=20 Å. The total exciton energy shifts to lower energies as the quantum wire radius increases. When the interface is sharp (abrupt), it varies from 2.97 eV (R=20 Å) to 2.81 eV, which corresponds to the blue color in the visible spectrum. Taking into account a graded interface 10 Å thick, the exciton energy is shifted towards higher energies. For a 20 Å wire radius, the exciton energy is 3.08 eV (violet).

The exciton energy blue shift due to the existence of a graded interface in the quantum wire is given by $\Delta E_{EXC}(R, \sigma) = E_{EXC}^0(R, \sigma) - E_{EXC}^0(R, \sigma = 0)$. Figure 2 depicts $\Delta E_{EXC}(R, \sigma)$ for $\sigma = 5$ Å, 10 Å, 15 Å. From this figure it is clear that graded interfaces represent an important factor to be taken into account if the wire radius is smaller than 50 Å. Even for an interface thickness of only 5 Å, the energy blue shift for R=20 Å is ∼50 meV. Effects related to the existence of graded interfaces can be neglected only for quantum wires with radius larger than 50 Å.

4   Conclusion

Remarkable interface related blue shifts on the exciton total energy in $In_{0.2}Ga_{0.8}N/GaN$ cylindrical quantum wires was shown to occur. These blue shifts are more pronounced for
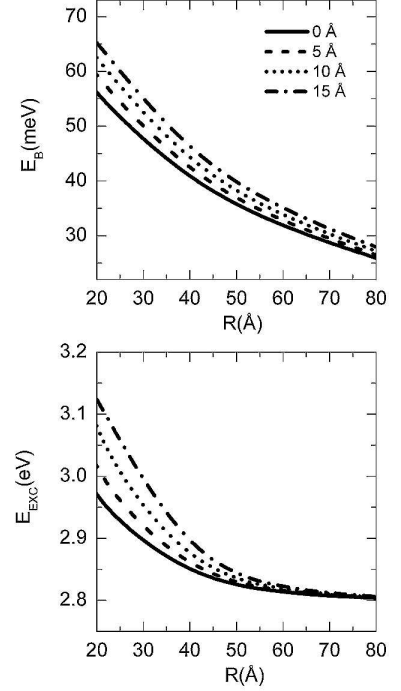

Figure 1. Shows the ground state binding (top) and total (bottom) ground state e-h confined exciton energy in $In_{0.2}Ga_{0.8}N/GaN$ quantum wires with interface thickness σ=0 Å (solid), 5 Å (dashed), 10 Å (dotted), and 15 Å (dotted dashed).

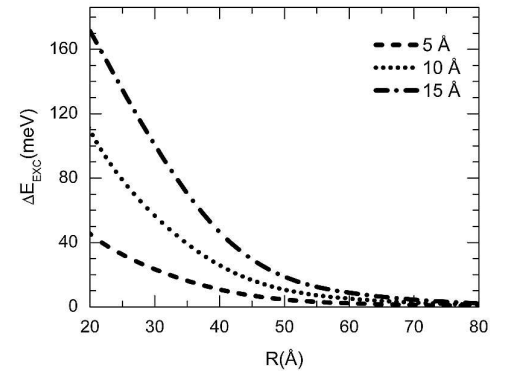Figure 2. Exciton energy blue shift $\Delta E_{EXC}(R, \sigma)$ in $In_{0.2}Ga_{0.8}N/GaN$ quantum wires with interface thickness 5 Å (dashed), 10 Å (dotted), and 15 Å (dotted dashed).

quantum wires with radius smaller than 50 Å, reaching values between 50 meV and 170 meV depending on the interface thickness and the wire radius. The enhancement of the confined exciton energy significantly enlarges the region of the visible spectrum spanned and must be taken into account for a better description of the optoelectronic properties of InGaN/GaN quantum wires.

A drawback of our calculations is that we have not taken into account the existence of an internal electric field due to

spontaneous and piezoelectric polarizations in wurtzite nitrides, which are highly important [8,9]. However, work is in development to include these fields in the confined exciton calculations in III-nitride based wires.

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