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Investigation of self-focusing effects in wurtzite InGaN/GaN quantum dots

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ABSTRACT

The third-order nonlinear optical properties in wurtzite InGaN/GaN pyramid and truncated-pyramid quantum dots are studied, and the oscillator strength, third-order nonlinear optical susceptibility and self-focusing effects are analyzed theoretically taken into account the strong built-in electric field effect due to the piezoelectric and spontaneous polarization in nitride materials. The numerical results clearly show that the quantum dot (QD) size of InGaN/GaN have a significant influence on the nonlinear optical properties of wurtzite InGaN/GaN quantum dots. Furthermore, the self-focusing effect increases with decrease in size of QDs.

1. Introduction

In recent years, III-nitride alloys have been the wide research subjects due to practical applications in the field of optoelectronic devices, high thermal conductivity, high electron-saturated drift velocity and small dielectric constant [1,2]. These materials have direct wide band gaps from 0.7 eV to 3.42 eV at room temperature, therefore, they are so useful in blue light emitting diodes industrial [3–5].

III–V nitride materials are founded in two different type structures: (i) wurtzite (WZ) [6] and, (ii) zinc-blend (ZB) [7]. In wurtzite structures, electronic states and optical properties are highly affected by the built-in electric field due to spontaneous (P_s) and piezoelectric (P_z) polarizations. The magnitude of the built-in electric field is estimated to be in the order of MV/cm. These properties do not exist in ZB structures, because they have high crystal symmetry [8–10]. Among III-nitride quantum dots (QDs) are already acknowledged as quantum nanostructures with high potentials in optoelectronic field; for instance, in light emitting diodes (LEDs), laser diodes (LDs), optical memories and single electron transistors [11–13].

In this nanometer scale semiconductors, the charge carriers (electrons and holes) are confined in all three dimensions [14,15] and due to the modification in the density of states, these quantum nanostructures are expected to exhibit enhanced optical nonlinearities and enhanced electro-optic effects. Indeed many of these optical nonlinear properties associated with intersubband transitions those due to large dipole transition and very large oscillator strength, these optical intraband nonlinear are large too. As the intrasubband dipole length extend over the QDs which are in nanometer ranges [16,17]. Compare to bulk semiconductors, QD semiconductors have larger third-order nonlinear susceptibility [18,19].

One of the most interesting effect associated with third order susceptibility (χ^3) is the self-focusing. It is typical type of nonlinear wave propagation that depends critically on the transverse profile of the beam. Self-focusing of the light is the process in which an intense beam of light modifies the optical properties of a material medium in such a manner that the beam is caused to come to a focus within or outside the material [20].

In this paper in order to understand the optical nonlinearity in QDs and its application as self-focusing effects, first we assume two different shapes of wurtzite $In_xGa_{1-x}N$ QDs (pyramid and truncated pyramid), then we calculated the Schrödinger equation in presence of the built-in polarization electric field in the framework of the envelope function, and the effective mass theory. The third-order nonlinear susceptibility of the taken QDs as function of DQ's size is investigated. Finally, the effects of QD size and shape on self-focusing effects have been analyzed.

2. Theoretical model

To model the device, two pyramid and truncated-pyramid shaped InGaN wurtzite QDs embedded in GaN material are assumed. The proposed structure has been shown in Fig. 1.

In order to study the electronic structures, different methods have been experienced [21–24]. The single band method is used

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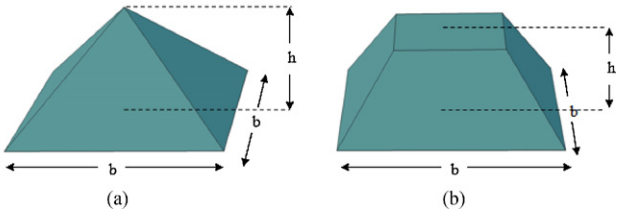

Fig. 1. The proposed pyramid (a) and truncated-pyramid (b) shaped InGaN QD within GaN material.

in this study. In the framework of the envelope function, and the effective mass theory, the Hamiltonian can be written as [22]:

$$H = \frac{-\hbar^2}{2}\nabla\frac{1}{m^*(x,y,z)}\nabla + V(x,y,z) \tag{1}$$

In which m^* is the electron effective mass and is given by:

$$m^*(x,y,z) = \begin{cases} m^*_{\mathrm{InGaN}} & \text{in QD} \\ m^*_{\mathrm{GaN}} & \text{in barrier} \end{cases}, \tag{2}$$

and

$$V(x,y,z) = \begin{cases} 0 & \text{inside QD} \\ \Delta E_{\mathrm{C}}\,(\Delta E_{\mathrm{V}}) & \text{else} \end{cases}, \tag{3}$$

where ΔE_{C} (ΔE_{V}) is the conduction and valence bands discontinuity [25]:

$$\Delta E_{\mathrm{C}} = 0.7\left(m \times 6.13 + (1-m)\times 3.42 - m(1-m) - E_{g_0}\right)\ \mathrm{eV}, \tag{4}$$

where m notifies Al molar fraction in the $\mathrm{In}_m\mathrm{Ga}_{1-m}$NQD.

As the most optoelectronic system needs an applied electric field to operate and III-nitride based structures also has a strong built-in electric field, one has to take into account the total fields effect in the Hamiltonian:

$$H = \frac{-\hbar^2}{2}\nabla\frac{1}{m^*(x,y,z)}\nabla + v(x,y,z) + e\vec{F}\vec{r} \tag{5}$$

where $\vec{F}$ denotes both the external and built-in electric fields. It should be mentioned that III-nitrides in the wurtzite phase have a strong spontaneous and piezoelectric polarization. The abrupt variation of the polarization at the interfaces gives rise to large polarization sheet charges which creates the built-in electric field. Therefore, the optical properties of wurtzite AlGaN/GaN QDs are affected by the 3D confinement electrons and the strong built-in electric field. This causes the simulation of the systems extremely challenging task.

The built-in electric field which applied in the equations is [26]:

$$F_{\mathrm{d}} = \frac{L_{\mathrm{br}}(P^{\mathrm{br}}_{\mathrm{tot}} - P^{\mathrm{d}}_{\mathrm{tot}})}{\varepsilon_0(L_{\mathrm{d}}\varepsilon_{\mathrm{br}} + L_{\mathrm{br}}\varepsilon_{\mathrm{d}})} \tag{6}$$

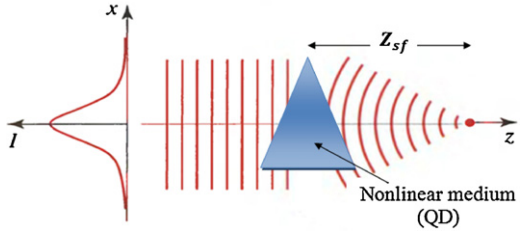

Fig. 2. A schematic QD nonlinear medium for self-focusing effect.

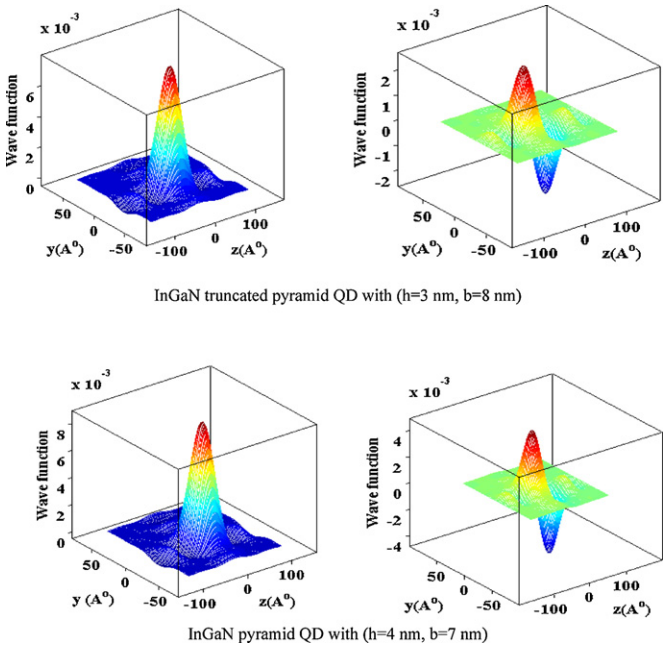

Fig. 3. The wavefunctions of the ground state and first excited state in InGaN pyramid, and truncated pyramid QDs. The wavefunctions are m^{-2} unit.

where $\varepsilon_{\mathrm{br}}$ (d) is the relative dielectric constant of the barrier (dot), $P^{\mathrm{br/d}}_{\mathrm{tot}}$ is the total polarization and $L_{\mathrm{br/d}}$ is the width of the barrier and height of the dot.

$$P^{\mathrm{br/d}}_{\mathrm{tot}} = P^{\mathrm{br/d}}_{\mathrm{piezo}} + P^{\mathrm{br/d}}_{\mathrm{sp}} \tag{7}$$

The piezoelectric polarization includes: one part induced by the lattice mismatch (ms), and the other caused by thermal strain (ts): $P^{\mathrm{br/d}}_{\mathrm{piezo}} = P^{\mathrm{br/d}}_{\mathrm{ms}} + P^{\mathrm{br/d}}_{\mathrm{ts}}$, where $P^{\mathrm{br/d}}_{\mathrm{ms}} = 2(e_{31} - e_{33}c_{13}/c_{33})\left((a-a_0)/a\right)$ and $P^{\mathrm{d}}_{\mathrm{ts}} = -3.2\times10^{-4}c/\mathrm{m}^2$ [26]. e_{31} and e_{33} are the piezoelectric coefficients, c_{31} and c_{33} are elastic constants, and 'a' is the lattice constant. All other material parameters can be found in [27].

To solve the Schrödinger equation, assuming that the wave functions are expanded in terms of the normalized plane waves [22]:

$$\psi_{\mathrm{nx,ny,nz}}(x,y,z) = \frac{1}{\sqrt{L_xL_yL_z}}\sum_{\mathrm{nx,ny,nz}} a_{\mathrm{nx,ny,nz}}\exp\, i(k_{\mathrm{nx}}x + k_{\mathrm{ny}}y + k_{\mathrm{nz}}z) \tag{8}$$

where $k_{\mathrm{nx}} = k_x + n_xK_x$, $k_{\mathrm{ny}} = k_y + n_yK_y$, $k_{\mathrm{nz}} = k_z + n_zK_{zs}$ and $K_x = 2\pi/L_x$, $K_y = 2\pi/L_y$, $K_z = 2\pi/L_z$. L_x, L_y and L_z are lengths of the unit cell along the x, y and z directions. n_x, n_y and n_z are the number of plane waves along the x, y and z directions respectively.

As reported in [28], the attraction of the normalized plane wave approach is the fact that there is no need to explicitly match the wave function, across the boundary of the barrier and QD. Hence this method is easy to apply to an arbitrary confining potential problem. As more plane waves are taken, more accurate results are achieved. We used thirteen normalized plane waves in each direction to form the Hamiltonian matrix (i.e. n_x, n_y and n_z from -6 to 6) and we formed 2197×2197 matrix. It was found that using more than 13 normalized plane waves in each direction takes significantly long computational time and only about 1 meV more accurate energy eigenvalues. By substituting the Eq. (8) in Schrödinger equation, eigenfunctions and eigenvalues are calculated.

To study the nonlinear optical absorption coefficient and refractive index, one has to know the third-order nonlinear susceptibility