

# Simulation of the Quantum-Confined Stark Effect in a Single InGaN Quantum Dot

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**Abstract** — By means of a 3D self-consistent numerical simulation we have calculated the effect of an externally-applied lateral electric field upon a single InGaN quantum dot. Overall, good agreement between the modeling and experimental results was observed. Modeling results support the observation that the quantum-confined Stark effect has both permanent dipole moment and polarizability components.

## I. INTRODUCTION

Semiconductor quantum dots (QDs) are zero-dimensional nanostructures that display properties analogous to those of atoms, such as discrete energy levels and the quantum-confined Stark effect (QCSE) [1,2]. Understanding the QCSE is important from both fundamental physics and device applications perspectives. Studying the exciton Stark shift permits a greater insight into the QD charge distribution, while the QCSE has found applications in ultrafast optoelectronic devices such as electro-optical modulators.

A number of studies characterizing the QCSE in single self-assembled QDs have shown that the application of an external electric field in the lateral direction permits control of the exciton wavefunction via the QCSE. III-nitride QDs (e.g. InGaN) [3] are particularly interesting as they possess built-in electric fields and high exciton binding energies, which are not found in the widely-studied III-arsenide family of QDs. Also QCSE has been extensively modeled in III-arsenide QDs [4], but not in III-nitride QDs.

We have previously studied the QCSE in single InGaN QDs using time-integrated microphotoluminescence ( $\mu$ PL) techniques [5]. In this paper we extend this experimental work by modeling the system using *nextnano*<sup>3</sup> [6], a nanostructure simulator capable of solving the self-consistent 3D nonlinear Poisson-Schrödinger equation. We employ a multi-band  $\mathbf{k}\cdot\mathbf{p}$  model to calculate the electron and hole probability densities inside the QD. Results from the modeling provide an insight into the mechanisms responsible for the PL emission.

## II. INGAN QUANTUM DOT MODEL

The InGaN QD sample was grown by metal-organic vapor phase epitaxy [3]. About 10 monolayers of InGaN were grown on 2.8- $\mu\text{m}$ -thick GaN templates, with QDs formed on

this layer capped by 7 nm of GaN. The In content was estimated to be approximately 20%. Pairs of Al electrodes with a separation of 1  $\mu\text{m}$  were fabricated on the surface [5].

The QDs were modeled as hexagonal pyramids of diameter 8 nm and height 2 nm, as shown in Fig. 1(a). When these parameters were incorporated into the *nextnano*<sup>3</sup> model, assuming uniform In alloy profile inside the QD and that In content of the QD and wetting layer were equal, the modeled exciton recombination energy agreed well with PL measurements. Comparison of the energy states between a QD in Ref. [7] (similar QD) and our model revealed a discrepancy of  $\sim 2\%$ . Self-consistent calculations involved the following steps: 1) Calculate the strain. 2) Calculate the piezoelectric charges from the strain and pyroelectric charges. 3) Solve the Poisson equation including piezoelectric and pyroelectric charges to obtain the electrostatic potential. 4) Solve the Schrödinger equation from the resulting electrostatic potential. The fully strained QD was simulated by minimization of the elastic energy within a continuum model approach that takes into account the symmetry of the hexagonal crystal structure.

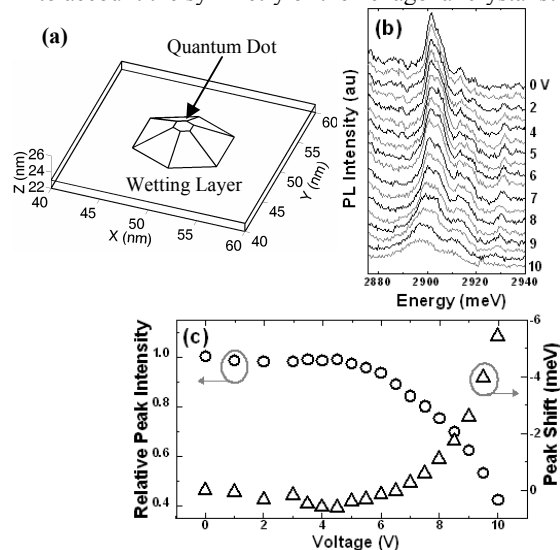


Fig. 1. (a) Geometry of the QD. (b) Series of  $\mu$ PL spectra recorded sequentially with increasing externally-applied voltage, from 0 to 10 V. The integration time was 10 s in each case. (c) Plots of relative peak intensity and peak shift as a function of applied voltage for the  $\mu$ PL spectra shown in (b). Experimental data from [5].

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In calculating the probability densities the program utilized a one-band model for the electrons and a six-band  $\mathbf{k}\cdot\mathbf{p}$  Hamiltonian for the holes. This could be justified as GaN and InN both have large band gaps and therefore the coupling between the conduction and valence bands could be neglected. The shift and splitting of the band edges due to strain were automatically included in these Hamiltonians by using the relevant deformation potentials. In addition, we assumed that the probability density was finite beyond the QD region. This was done by using Dirichlet boundary conditions for the Schrödinger equation beyond the QD boundaries.

### III. RESULTS

Details of the experimental setup can be found in Ref. [5]. Figure 1(b) shows a series of consecutively-recorded  $\mu\text{PL}$  spectra from the QD with increasing lateral field strength. In the absence of an electric field, the spectrum exhibited a narrow peak originating from exciton recombination. However as the voltage was increased from 0 to 10 V, the PL peak red shifted, declined in intensity and the linewidth increased. Figure 1(c) plots the relative peak intensity and the peak shift as a function of the applied voltage. A peak shift of  $\Delta E = 5.4 \text{ meV}$  was observed at 10 V. Modeling with ATLAS (Silvaco International) calculated that a 10 V bias applied across the  $1 \mu\text{m}$  electrodes gap corresponded to a mean field of  $10 \text{ MVm}^{-1}$  at the QD, mostly parallel to the QD layer.

The effect of the external field was modeled using *nextnano*<sup>3</sup>. Increasing the electric field caused the conduction and valence bands to ‘tilt’ along the direction of the electric field, as shown in Fig. 2(a). As a result this changed the electron and hole energy levels and caused a shift in PL energy as presented in Fig. 2(b). The simulation calculated a peak shift of  $\Delta E = 5.9 \text{ meV}$ . This is in good agreement with the experimental result, given the simplifications employed in the modeling (such as neglecting the effects of residual doping or charged defects). Also the exact dimensions of the QD are not known, and these would also influence the size of  $\Delta E$ . The peak shift  $\Delta E(F)$  due to the QCSE can be expressed as:

$$\Delta E = \mu F - \alpha F^2 \quad (1)$$

where  $F$  is the external electric field,  $\mu$  and  $\alpha$  are the components of the permanent dipole moment and the polarizability in the electric field direction. Curve fitting of the result in Fig. 2(b) yields values of  $\mu \sim 1.0 \times 10^{-29} \text{ Cm}$  and  $\alpha \sim 1 \times 10^{-35} \text{ Jm}^2\text{V}^{-2}$ . These compare well with the experimentally measured values [5]. The non-zero  $\mu$  is consistent with measurements in other III/V QDs, and indicates that the lateral permanent dipole moment is significant [8].

Visualization of the electron and hole probability densities, as shown in Fig. 2(c)-(f), explains the decline in the PL intensity with increasing electric field. The electric field ‘tilts’ the bands and causes the electron and hole probability density to shift in opposite directions. This leads to a decrease in the overlap between the electron and hole wavefunctions, and consequently a reduction in the oscillator strength.

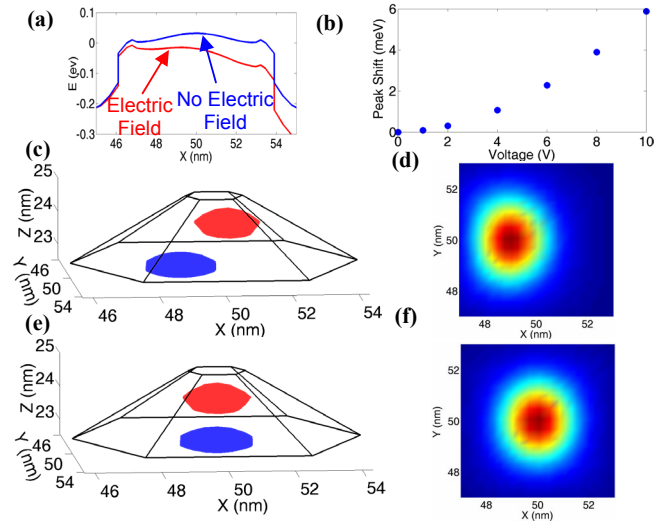


Fig. 2. (a) ‘Tilt’ in the valence band due to the electric field along the  $x$  axis. Modeled red shift in the PL due to applied bias (b). Visualization of the electron (red) and hole (blue) probability (80%) (c) and hole probability at  $z = 23 \text{ nm}$  (d) in the presence of  $10 \text{ MVm}^{-1}$  lateral electric field. Same visualization with no electric field (e, f).

### IV. CONCLUSION

We have calculated the wavefunctions and energies of the lowest states in an InGaN QD with an externally applied lateral electric field by means of a 3D numerical simulation. Modeling supports the experimental observation of a redshift in the exciton energy and field dependence expressed by  $\Delta E = \mu F - \alpha F^2$ . It also demonstrated that the decrease in PL intensity, with increasing field, was due to the decrease in the overlap between the electron and hole wavefunctions.

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