Modeling the optical properties of nitride nanostructures – InGaN quantum dots and coupled asymmetric GaN/AlGaN quantum discs

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III-nitride nanostructures (e.g. InGaN) are particularly interesting as they posses large built-in electric fields and high exciton binding energies. By means of 3D numerical simulations using the next**nano**[3] software, we have calculated the effect of an externally applied lateral electric field upon a single InGaN quantum dot (QD), and the electronic states in coupled asymmetric GaN/AlGaN quantum discs of MBE grown nanocolumn heterostructures. Overall, good agreement between the modeling and experimental results was observed.

For the QDs, the modeling results support the observation that the quantum confined Stark effect (QCSE) has both permanent dipole moment and polarizability components. 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. Applying an external electric field in the lateral direction 'tilts' the conduction and valence band edge confinement potentials along the direction of the electric field (Fig. 1 (a)) and thus permits control of the exciton wave function via the QCSE. The QD was modeled as a hexagonal pyramid of diameter 8 nm and height 2 nm as shown in Fig. 1 (e) with a uniform indium distribution (20 %) in the QD and in the wetting layer. The calculated exciton recombination energy (2.9 eV) agreed well with photoluminescence (PL) measurements. The experimental results [1] for the exciton peak of the QD with increasing lateral field strength are shown in Fig. 2. As the voltage was increased from 0 V to 10 V, the PL peak red shifted and declined in intensity due to a reduced electron-hole wave function overlap as the electron and the hole move into opposite directions (Fig. 1 (c) vs. Fig. 1 (e)).

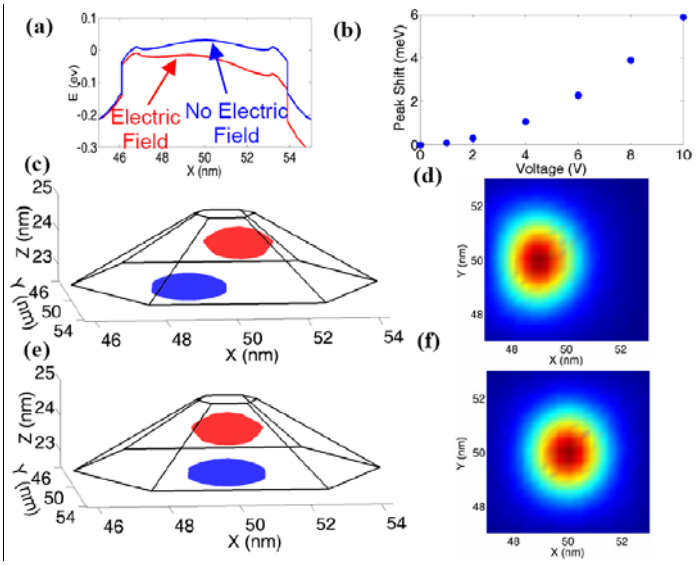

Fig. 1: *(a) 'Tilt' in the valence band edge due to the lateral electric field along the x axis. (b) Modeled red shift in the photoluminescence due to applied bias. (c) Visualization of the electron (red) and hole (blue) probability amplitudes (80 %) and (d) slice of the hole probability amplitude at z=23 nm in the presence of 10 MV/m lateral electric field. (e), (f) Same visualization without lateral electric field.*

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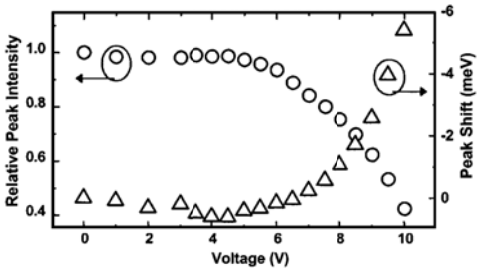

Fig. 2: *Plots of relative peak intensity and peak shift (red shift) for a series of μPL spectra recorded sequentially with increasing externally applied voltage, from 0 V to 10 V [1]. The peak shift is well reproduced by the numerical calculations shown in Fig. 1 (b).*

From a technological point of view, growing nitride heterostructures is either expensive when using GaN substrates or leads to defects in the structure (and thus reduced device performance) when using lattice mismatched SiC or sapphire substrates. An attractive solution would be the ability to grow defect free on cheap Si substrates, as is in fact the case for self-assembled nanocolumn heterostructures grown by plasma assisted MBE. For this reason, we have investigated coupled asymmetric GaN quantum discs (Q-discs) in order to gain insight into the carrier dynamics of these structures. Our quantum well like Q-discs are grown at the tip of GaN nanocolumns and are separated by thin $Al_{0.5}Ga_{0.5}N$ barriers of width 1 nm. The discs have a diameter of 100 nm and a height of 4 nm (labeled 'DA') and 3 nm ('DB'), respectively. Fig. 3(a) shows the calculated conduction and valence band edges along the growth direction ([0001] axis) together with the two lowest electron and hole energies. The calculated emission energies of the discs DA and DB are 3.47 eV and 3.58 eV. The calculations show that the tunneling of electrons from DB to DA is possible, as the electron energy of DB lies above the triangular potential of the DA energy state. However, the converse is not true as the electron energy in DA is lower (by ~0.1 eV) and lies within the triangular region of the confinement potential, implying stronger localization. Fig. 3 (b) shows the that the ground state of the electron in Q-disc DB tunnels through the AlGaN barrier and extends into DA. Hence, even under nonresonant condition, there is evidence of weak coupling between the Q-discs. These modeling results were used to interpret time-resolved and time-integrated PL measurements of the DA and DB peaks as a function of excitation power where free carrier screening of the built-in piezo- and pyroelectric fields was observed leading to different blue shifts in the emission energy for DA and DB.

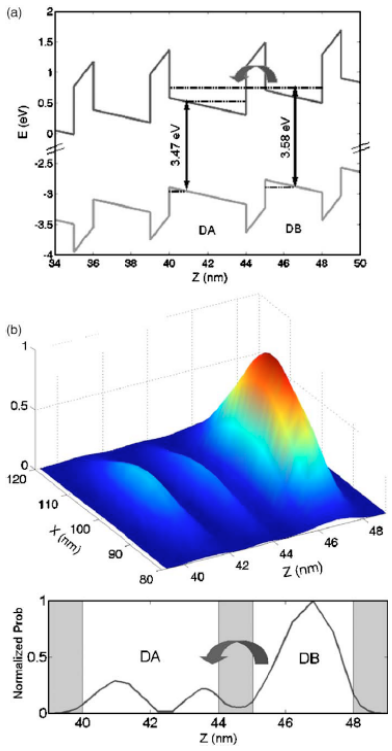

Fig. 3: *(a) Band diagram for electrons and holes. (b) Calculated electron wave function showing that the DB ground state extends into DA, giving rise to the possibility of tunneling from DB to DA.*

[1] J. W. Robinson et al., Appl. Phys. Lett. **86**, 213103 (2005)