Optoelectronic properties of a GaN quantum dot grown on a $Al_{0.5}Ga_{0.5}N$ $(11\bar{2}2)$-orientated surface

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The electronic and optical properties of a semi-polar orientated quantum are investigated by experimental and theoretical means. These GaN nanostructures are grown by molecular beam epitaxy on $Al_{0.5}Ga_{0.5}N$ $(11\bar{2}2)$-oriented surfaces using ammonia (NH_3) as a nitrogen precursor. The fabrication sequence of the nanostructures is as follows: (i) A two-dimensional GaN layer is grown; (ii) The GaN surface is held under an ammonia (NH_3) flux; and finally (iii) Three-dimensional islands are formed via a surface morphology transition by switching off the NH_3 flux. The samples consists of three GaN planes covered by a 30 nm thick $Al_{0.5}Ga_{0.5}N$ layer, followed by a fourth uncovered nanostructure plane for characterization by atomic force microscopy. Depending on the quantity of GaN deposited a modification of the nanostructure shape is observed. For small amounts (< 1.6 nm) the surface morphology is dominated by the presence of isolated islands; whereas, for larger amounts, ~ 1.6 to ~ 4.3 nm, the morphology evolves toward elongated nanostructures aligned along the $[1\bar{1}00]$ direction [1]. Their optoelectronic properties are investigated by means of a standard 8×8-band $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian. The modification applied to the wave-function generating kernel is a unitary transformation to the observed crystallographic orientation. In the two-dimensional case considered here, $x \parallel [\bar{1}\bar{1}23]$ and $y \parallel [11\bar{2}(3\lambda)]$ where $\lambda = (a/c)^2$, with $a : c$ being the ideal ratio of the substrate. The scheme is applied to a single isolated quantum dot. The elastic energy arising from the $GaN/Al_{0.5}Ga_{0.5}N$ lattice mismatch is minimised and the band structure is calculated (for the Γ conduction band, and HH, LH, and Δ_{so} valance bands). The built-in electric polarization, aligned parallel to the c-direction, is found to dominate the physics of the quantum dot [1]. That, combined with the quantum dot morphology, influences the position of the $+/-$ peaks of the electrostatic field and their magnitude; (*ie.* a reduction in the quantum confined Stark effect is found, and the conduction/valance bands are affected accordingly. In particular, for this case, valance-band states are strongly localized at the rhs. of the quantum dot (at $\max[V^-]$), whereas conduction-band states (at $\max[V^+]$) are localised along the surface on the opposite of the quantum dot. These observations are found to persist at finite temperatures in the simulated and experimental range, $[5, 300]$ K. In all cases, electron and hole states are confined to the quantum dot area allowing for the possibility of high luminescence efficiency [2] from these semi-polar nanostructures.

References

[1] A. Kahouli *et al. J. Appl. Phys* **110**, 084318 (2011).

[2] G. Jurczak and T. D. Young. *Applied Surface Science*, In press (2012).

Supplimentary page

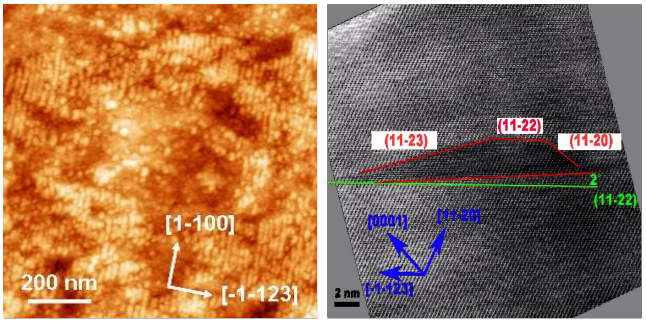

Figure 1: Image obtained by experimnental observation of GaN nanostructures grown on $Ga_{0.5}Al_{0.5}N$ $(11\bar{2}2)$. Left: By atomic force microscopy. Right: By transmission electron microscopy.

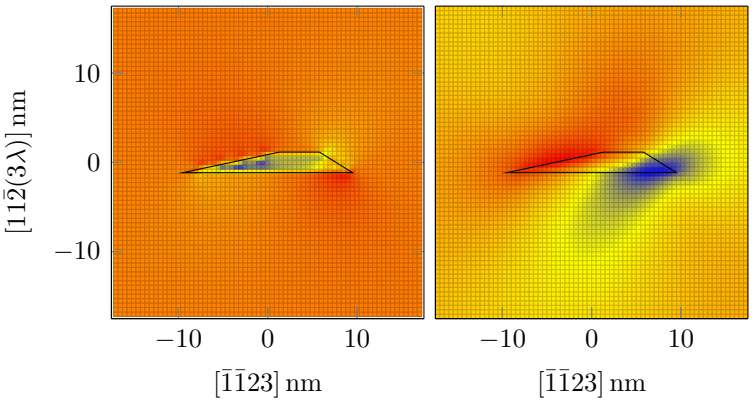

Figure 2: Surface plot of the classical fields arising in the quantum dot area using a "hot" colour map. Peaks are aligned parallel to the c-axis. Left: Spherical components of the strain field. Right: The induced electrostatic potential.

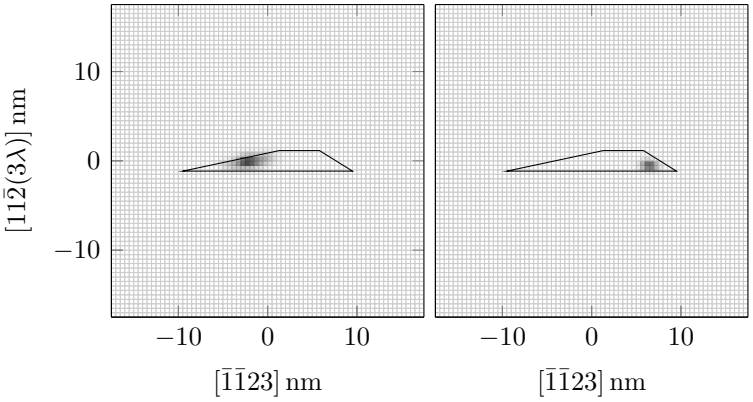

Figure 3: Probability amplitudes obtained from diagonalising of the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian using a "grayscale" colour map. Confinement of states to the quantum dot is evident; *cf.* Fig. 2. Left: Γ conduction band (electron). Right: HH valance band (hole).