

Theory of Strain, Built-in Electric Fields and Carrier States in Self-Organised GaN/AlN QDs

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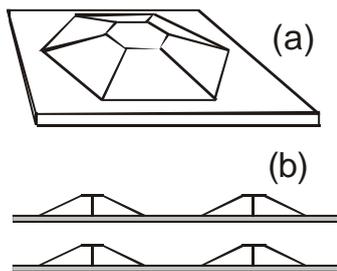
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We present a theory of the electronic structure of GaN/AlN quantum dots (QDs), including built-in strain and electric field effects. A novel Green's function technique is developed to calculate the 3D strain distribution in semiconductor QD structures of arbitrary shape and of wurtzite (hexagonal) crystal symmetry. We derive an analytical expression for the Fourier transform of the QD strain tensor, valid for the case when the elastic constants of the QD and matrix materials are equal. A simple iteration procedure is described which can treat differences in the elastic constants. An analytical formula is also derived for the Fourier transform of the built-in electrostatic potential, including the strain-induced piezoelectric contribution and a term associated with spontaneous polarization. The QD carrier spectra and wave functions are calculated using a plane-wave expansion method we have developed, and a multi-band $\mathbf{k}\mathbf{p}$ model. The method used is very efficient, because the strain and built-in electric fields can be included analytically through their Fourier transforms. We consider in detail the case of GaN/AlN QDs in the shape of truncated hexagonal pyramids shown in Fig.1. We present the calculated 3D strain and electrostatic potential distributions (see Fig.2), the carrier spectra and wave functions in the QDs. Due to the strong built-in electric field, the holes are localized in the wetting layer just below the QD bottom, while electrons are pushed up to the pyramid top. Both also experience an additional lateral confinement due to the built-in field. We examine the influence of several key factors on the calculated confined state energies. Use of a one-band, effective mass Hamiltonian overestimates the electron confinement energies by ~ 100 meV, because of conduction band non-parabolicity effects. By contrast, a one-band valence Hamiltonian provides good agreement with the calculated multi-band ground state energy. Varying the QD shape has comparatively little effect on the calculated levels (see Fig.3), because of the strong lateral built-in electric field. Overall, the transition energies depend most strongly on the assumed built-in electric field. Finally, the energy of the ground optical transition in GaN/AlN QDs is compared with available experimental data [1] and good agreement is found between theory and experiment (Fig 4).

References

[1] F. Widmann, J. Simon, B. Daudin, *et.al.*, Phys. Rev. B, **58**, 15989 (1998)



Figures

Fig.1 Showing schematic diagrams of considered GaN/AlN QDs shaped as truncated hexagonal pyramids (a) 3D view of a single QD standing on a wetting layer; and (b) view of the QD structure in the x-z plane.

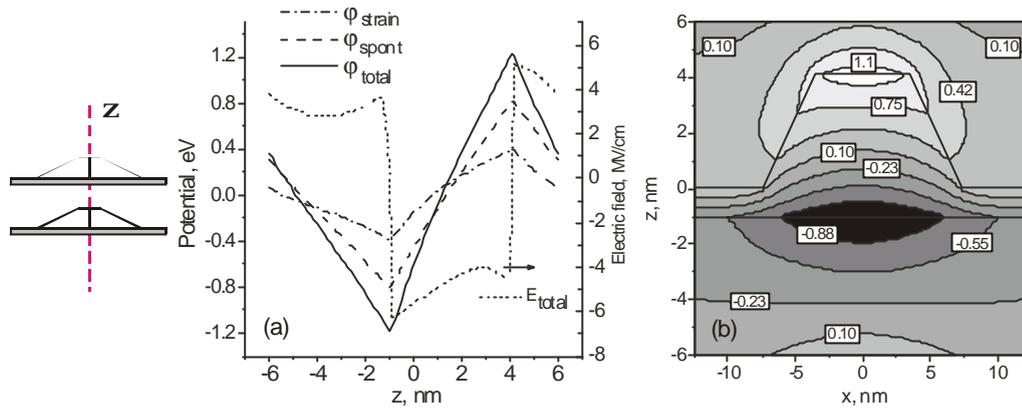


Fig.2. (a) Calculated variation of the built-in electrostatic potential components, and total electric field, E , along the (0001) direction ($x=y=0$). Solid line: Total built-in electrostatic potential, ϕ_{total} , found as the sum of the strain-induced piezoelectric potential, ϕ_{strain} , (dot-dashed line) and the spontaneous polarization term, ϕ_{spon} (dashed line). (b) Contour plot of the variation in the total built-in electrostatic potential, ϕ_{total} in the x - z plane ($y=0$). The darkest areas show regions of low potential (where holes are trapped), and the brighter areas regions of higher potential (where electrons are trapped). The numbers in boxes show the magnitude of the potential (in eV) along the different contour lines.

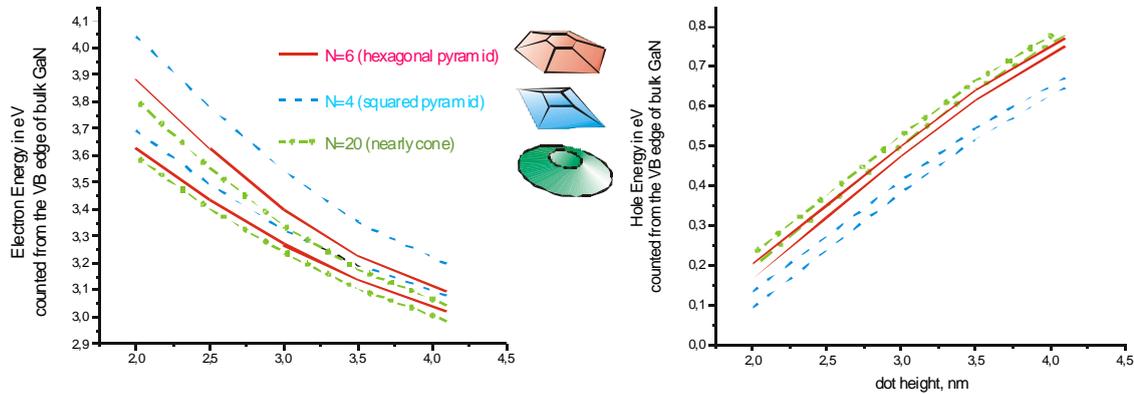


Fig.3 Variation of the electron and hole energy levels with QD height for different QD shapes

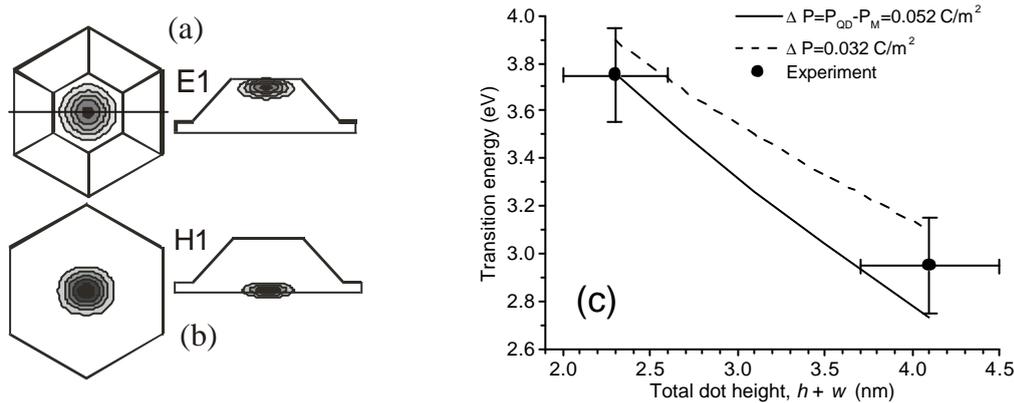


Fig.4 Probability density distribution, $|\psi(\mathbf{r})|^2$ for the first electron (a) and hole (b) states in the GaN/AlN QD in the shape of truncated hexagonal pyramid. (c) Calculated dependence of the ground state transition energy $E1-H1$ on QD height for different assumed values of the spontaneous polarization difference. Black dots with error bars: experiment [1]; solid line: using spontaneous polarization values for GaN, P_{QD} , and AlN, P_M , calculated by Bernardini, et.al. [Phys. Rev. B, **56**, 10024 (1997)]; dashed line: using smaller values of spontaneous polarization reduced by $\sim 40\%$, consistent with previous analysis of GaN/AlGaIn quantum well structures [M. Leroux, et.al., Phys. Rev. B., **58**,13371 (1998)]