Competing Effects of Piezoelectric and Pyroelectric Polarization in GaN/AlN Quantum Dots: Multimillion-Atom $sp^3d^5s^*$ Tight-Binding Simulations

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INTRODUCTION

Wide-bandgap GaN/AlN heterostructures are promising for applications in ultraviolet (UV) light emitting optoelectronic devices [1]. These structures exhibit large spontaneous and strain-induced polarization, which have significant effects on their electronic and optical properties. In this work, using a 20-band $sp^3d^5s^*$ tight-binding framework in NEMO 3-D [2], we calculate the electronic and optical properties of GaN/AlN quantum dots.

SIMULATION MODEL

Based on the atomistic valence-force field (VFF) and a variety of tight-binding models, NEMO 3-D enables the computation of atomistic strain fields and electronic structure in materials containing over 1 billion atoms. Excellent parallel scaling up to 32,000 cores has recently been demonstrated. The piezoelectric charge density is derived by taking divergence of the polarization. The induced potential is determined by the solution of 3-D Poisson equation in the Wurtzite lattice.

DISCUSSION

The GaN/AlN quantum dot contains ~3 million atoms and of truncated pyramidal shape having a height and base length of 3 nm and 22 nm, respectively (Fig. 1). Strain is found (Fig. 2) to be long-ranged and penetrate around 16 nm into the dot substrate and 6 nm in the capping layer. The induced built-in potentials are shown in Fig. 3. It is seen that, in contrast to the well-studied InN/GaN system [3], the pyroelectric potential is significantly larger and *adds* to the piezoelectric counterpart. Fig. 4 shows the topmost valence and the first four conduction band wavefunctions (on the X-Y plane) as a function of 1) interface and fundamental atomistic symmetry, 2) strain relaxation, 3) piezoelectric, and 4) pyroelectric fields—all resulting in shift in energy spectrum. Also noticeable are the deformed valence band, conduction band P-level anisotropy and non-degeneracy, and formation of mixed orbitals. Fig. 5 shows the influence of the internal fields on the bandgap. One can see that, while the red-shift due to the strain relaxation and the piezoelectric potential is moderate (~0.42eV), the effect of pyroelectricity is significantly larger (~1.5eV). Fig. 6 shows the inter-band optical transition rates in the quantum dot, revealing significant suppression and strong polarization anisotropy due to spatial irregularity (rotation) in the wavefunctions.

CONCLUSION

In contrast to the well-studied InN/GaN system, the peak pyroelectric potential is *4 times larger* than the piezoelectric counterpart and results in a significant reduction (redshift) in the electronic bandgap (quantum confined stark effect) near the Brillouin zone center, pronounced non-degeneracy in the excited state, and strongly modulated optical transition rates.

ACKNOWLEDGEMENT

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REFERENCES

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[2] G. Klimeck, et al., *IEEE Trans. on Elect. Dev.*, vol. 54, 9, pp. 2079–99, 2007.
[3] S. Ahmed, et al., *IEEE Trans. on Elect. Dev.*, vol. 57, 1, pp. 164–173, 2010.

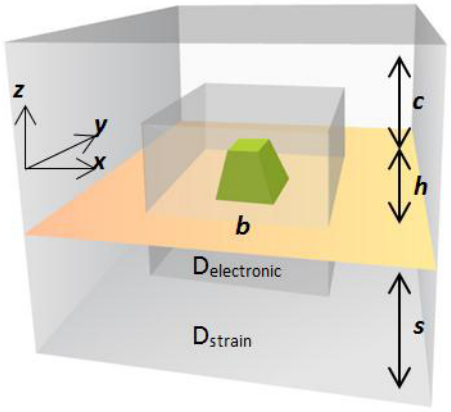

Fig. 1. Simulated truncated pyramidal GaN/AlN QD.

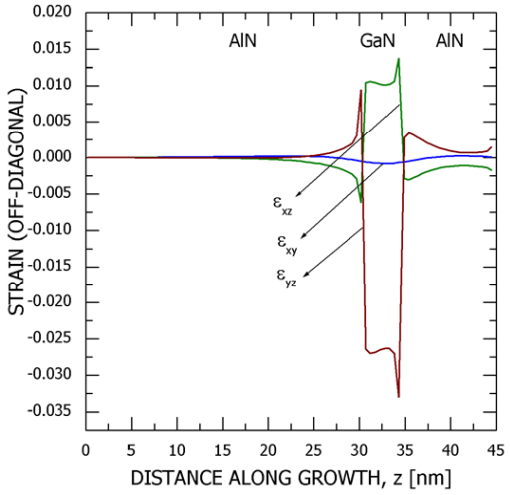

Fig. 2. Diagonal strain profiles in the growth direction.

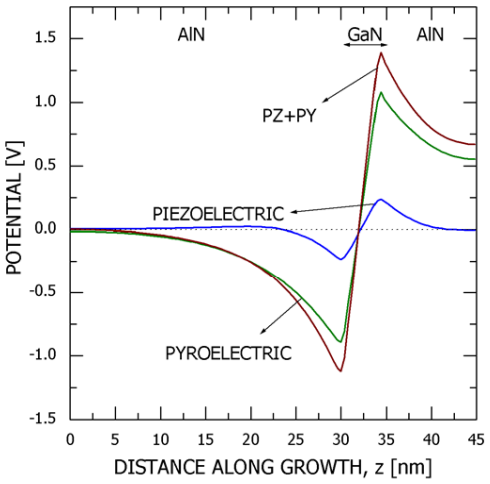

Fig. 3. Built-in potential profiles in the growth direction.

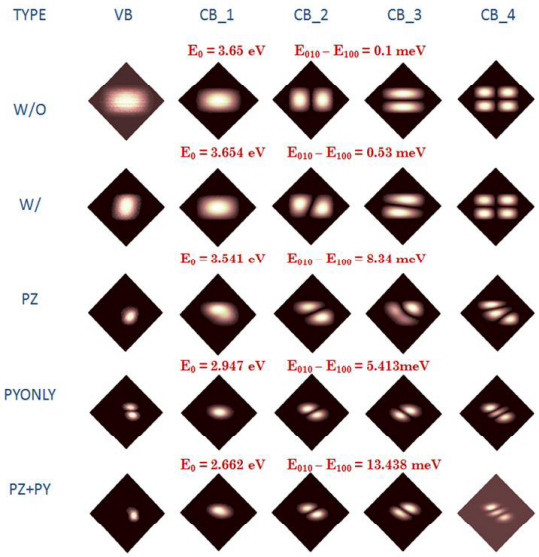

Fig. 4. Wavefunctions due to the internal fields.

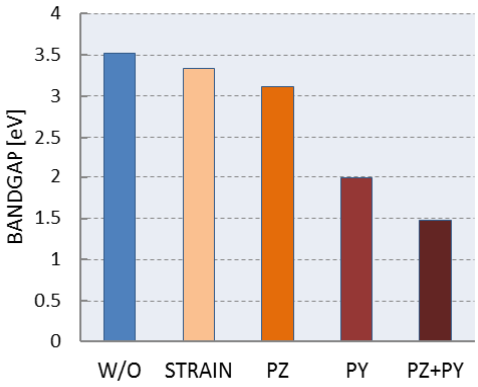

Fig. 5. Bandgap as a function of the internal fields.

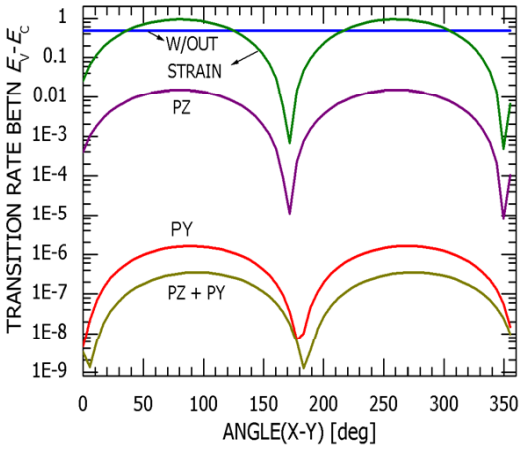

Fig. 6. Optical transition rates due to the internal fields.