GaN/InGaN/GaN Disk-in-Wire Light Emitters: Polar *vs.* Nonpolar Orientations

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INTRODUCTION

Nanoscale InGaN heterostructures are promising candidates for efficient, full-spectrum optical emitters and for use in conventional (e.g. lasers, solid-state lighting) as well as novel (e.g. near-field photolithography, single phonon based quantum cryptography, diagnostic medicine and biological imaging) applications. However, when grown along the [0001] polar axis, these structures exhibit large polarization fields, which significantly affect their electronic and optical properties and lead to poor internal quantum efficiency (IQE). Recently, for *larger* (mainly quantum well based) structures, it has been demonstrated that IQE could improve, if grown in the non-polar crystallographic orientations (such as *m*-plane or *a*-plane) [1]. This work aims to computationally investigate the validity of some of these claims, and in particular, for recently reported reduced dimensionality *disk-in-wire* structures [2].

SIMULATION MODEL

The overall simulation strategy is based on our in-house QuADS 3-D computational platform. Here, first, to compute the electronic structure and the interband optical transition rates, we have employed a 10-band sp^3s^* tight-binding framework as available in the NEMO 3-D software toolkit [3][4]. However, extensions have been made, where the crystallographic orientation for the non-polar *m*-plane structure is described via appropriate rotations in the lattice vectors. Strain and the polarization fields have been calculated via a coupled atomistic valence-force field (VFF) and 3-D Poisson solver. Finally, the microscopically determined optical transition parameters are incorporated into a TCAD toolkit to obtain the terminal characteristics and *compare* how atomicity and the net polarization field affect the IQE of these two systems.

RESULTS AND DISCUSSION

The *c*-plane and the *m*-plane GaN/InGaN/GaN disk-in-wire structures both have height and base length of 100 nm and 14 nm, respectively, and contain ~10M atoms. The undoped $In_{0.25}Ga_{0.75}N$ quantum disk is positioned at the center of the GaN nanowire and has a thickness of ~3 nm. The calculated built-in potentials are shown in Fig. 1. While, in both systems, the pyroelectric contribution is negligible (not shown here), the piezoelectric component is still significantly large and *atomistically* symmetric in nature. However, the magnitude of the net potential for the *m*-plane structure is *reduced* by ~36.7 mV as compared to the *c*-plane counterpart. Fig. 2 shows the wavefunctions for three cases: w/out internal fields, with strained lattice, and including net polarization fields. It is clear that, compared to *c*-plane, the *m*-plane structure exhibits increased HOMO-LUMO overlap as well as a larger bandgap (Fig. 3). This, in effect, results in a higher *average* interband transition rate (0.18 in the *m*-plane and 0.082 in the *c*-plane) and a greater degree of isotropy in the optical emission characteristic (Fig. 4). Finally, when coupled to the Synopsys' TCAD toolkit, all of these facts result in higher spontaneous emission and improved (along with a delayed *droop*) IQE characteristic (Fig. 5). To conclude, a GUI enabled educational version of the simulator (dubbed *nanoSSL* and shown in Fig. 6), which currently computes the electronic and optical transition properties, has been developed and made freely available on NSF's nanoHUB.org.

ACKNOWLEDGMENT

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REFERENCES

[1] P. Waltereit *et al.*, *Nature*, vol. 406, pp. 865–868, 2000.
[2] S. Deshpande *et al.*, *Nature Comm.*, vol. 4, number. 1675, DOI: 10.1038/ncomms2691, 2013.
[3] G. Klimeck, *et al*., *IEEE Trans. on Elect. Dev.*, vol. 54, 9, pp. 2079–99, 2007.
[4] S. Ahmed, *et al*., *IEEE Trans. on Elect. Dev.*, vol. 57, 1, pp. 164–173, 2010.

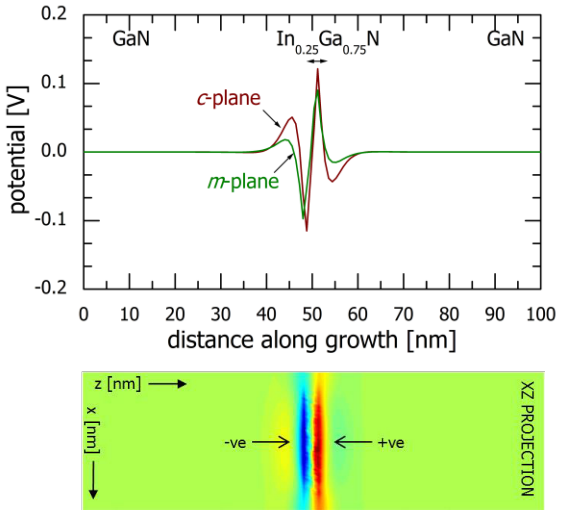

Fig. 1. Potential distributions in the growth direction.

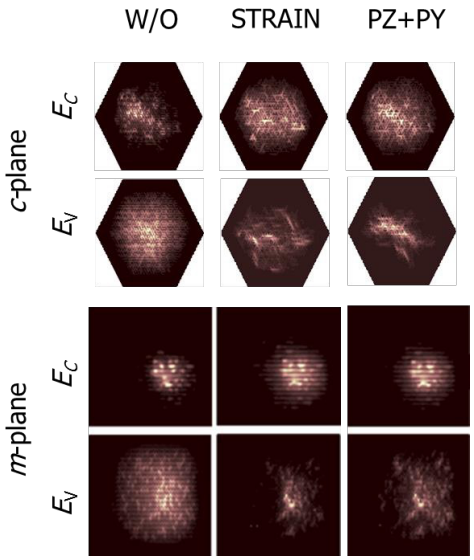

Fig. 2. Wavefunctions due to the internal fields.

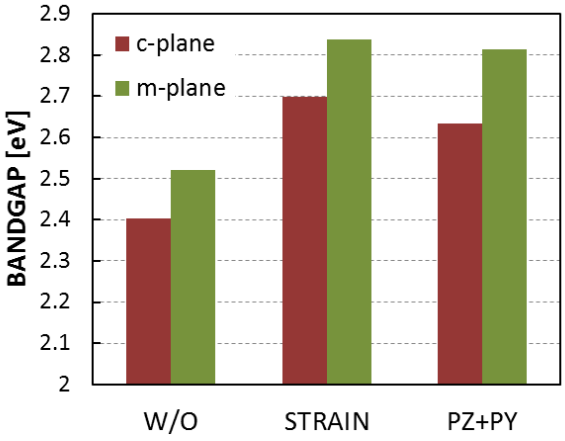

Fig. 3. Bandgap as a function of the internal fields.

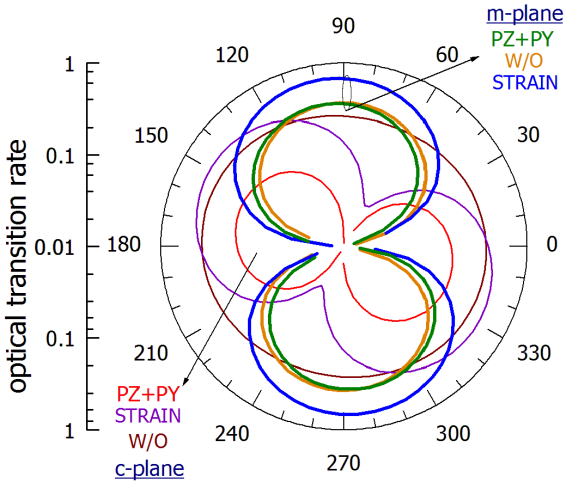

Fig. 4. Optical transition rates.

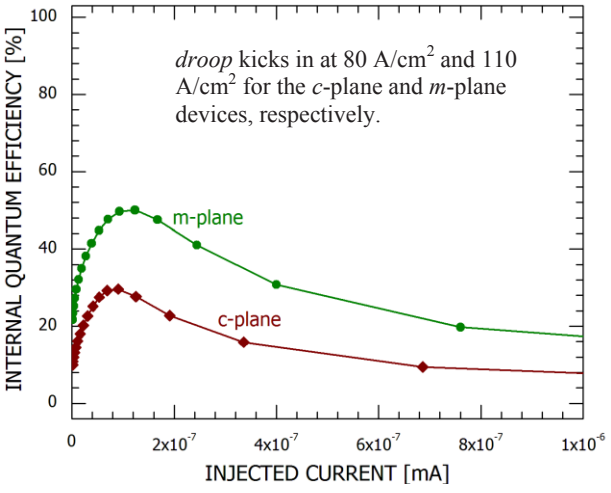

Fig. 5. IQE as a function of injected current.

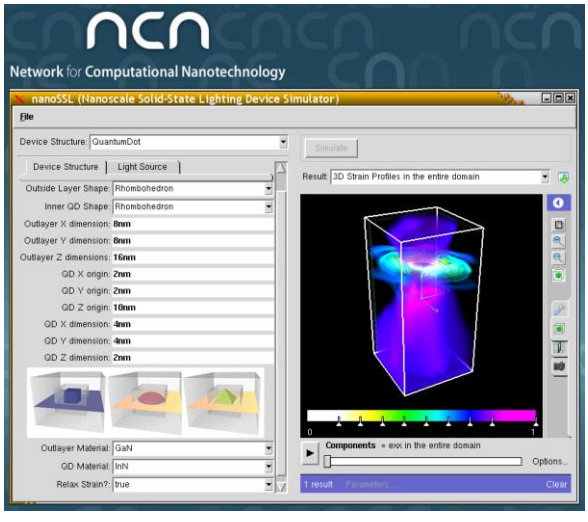

Fig. 6. *nanoSSL* simulator: https://nanohub.org/resources/nanossl.