# Physics-Based Simulation of a Core-Multishell Nanowire Light Emitting Diode.

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***Abstract*—We report on the computational analysis of a triangular core-multishell nanowire light emitting diode with three joint $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}$ active layers. The different crystal orientations of these layers lead to different polarization induced internal fields and transition energies. The simulation approach accounts for these effects by including the calculation of strained band edges and piezo potentials and provides a self-consistent model for the coupled 3D bulk and 2D quantized structure. The simulator is targeted to a comprehensive analysis of luminescence including the spatial variation of transition energies and carrier densities.**

## I. Introduction

Gallium nitride based light emitting diodes (LEDs) have evolved into powerful and highly efficient devices for solid state lighting over the past years [1]. These LEDs are grown by planar epitaxy on rather expensive sapphire and silicon carbide substrates having active $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}$ quantum well (QW) regions. A novel approach are nanowire LEDs which can be grown on inexpensive Si substrates and are expected to bridge the "green gap" by allowing a higher In content in the active region due to improved strain management. Recent implementations of nanowire LEDs include the nanocolumn LED with a quantum disk active region [2] and the core-multishell nanowire LED with a lateral shell type QW active region [3]. The large area active region of the latter design is expected to enable a high power density.

Though electroluminescence has been demonstrated for these devices the complex interaction between strain induced band gap changes, piezo polarization, and transport in bulk as well as lower dimensional regions aggravates the control of particular luminescence properties and/or high efficiency. This creates the need for physics based simulation of nanowire LEDs targeted to the design of the luminescence so that the current restrictions in the technical applicability are lifted.

In the scope of this work the properties of a core/shell type nanowire LED are analyzed. The subsequent sections depict the operation of the simulation framework used for the analysis and present simulation results for the core/shell nanowire LED followed by a brief discussion.

## II. Simulator

The device simulator implements a microscopic and coupled solver for computing transport and luminescence in photonic semiconductor devices with quantized regions [4], [5]. It has been successfully applied to the analysis of quantum disk nanowire LEDs [6]. The simulator operates on 1D, 2D, and 3D geometries with a focus on 3D.

Prior to the transport simulation, the strain induced band edge shifts and polarization charges are calculated. They are derived from the solution of the intrinsic strain based on a linear elasticity model. A six band wurtzite $\mathbf{k}\cdot\mathbf{p}$ calculation yields the valence band structure and the band edge shift due to strain. Drift/diffusion carrier transport is solved for bulk as well as for partially quantized carriers perpendicular to the quantization direction. This yields a varying number of continuity equations for each species: one 3D bulk continuity equation and as many 2D/1D continuity equations as there are QW and quantum wire regions within the structure. The different carrier populations are connected by capture through adding recombination terms to the respective continuity equations. All bound and unbound carrier populations are coupled by means of the Poisson equation. The carrier distribution in the direction of quantization is described by the single- or multi-band Schrödinger equation. The Schrödinger solver implements a predictor-corrector scheme to solve the coupled Schrödinger and Poisson equation selfconsistently. Luminescence spectra arise from the semiclassical theory including Coulomb interactions on a screened Hartree-Fock level.

## III. Core/shell nanowire LED

The core/shell nanowire LED [3] to be investigated has a triangular outline as depicted in Fig. 1. The $(0001)$ direction of the wurtzite crystal is in the direction of the y-axis of the model. The other sides are perpendicular to the $(1\bar{1}0\bar{1})$ and $(\bar{1}10\bar{1})$ direction yielding an almost equal-sided triangle. The LED has contacts on opposite faces of the cylinder. The n-contact is on the center triangle of one face and the p-contact is on the outer p-GaN surface of the opposite face.

The LED has three joint $\mathrm{In}_{0.09}\mathrm{Ga}_{0.91}\mathrm{N}$ 8 nm wide QWs parallel to each side. One QW is perpendicular to the c-axis of the crystal lattice while the other QWs are semipolar cutting the c-axis at an angle of about 30 degrees. Due to the strain anisotropy of the wurtzite crystal, the volumetric strain in the QW perpendicular to the c-axis yields -1.5% and -1.27% for the semipolar directions (see Fig. 2). The in-plane strain in the xz-plane, $\varepsilon_{\mathrm{xx}} + \varepsilon_{\mathrm{zz}}$ and the strain in the y-axis differ in their sign for the polar QW whereas the respective values of

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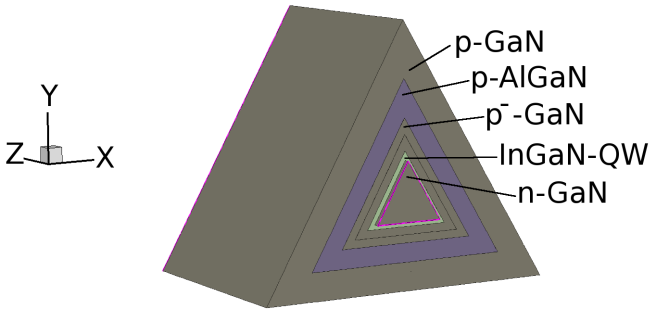


Fig. 1. Geometry of the core/shell nanowire LED. The triangular cylinder is 530 nm wide and 400 nm long.

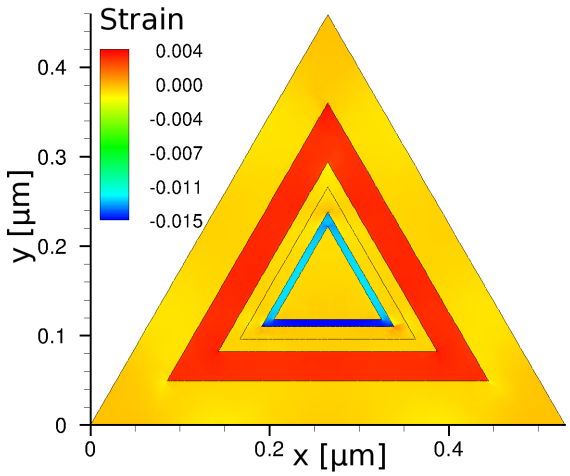


Fig. 2. Strain in a plane parallel to the triangular surface. The figure shows the trace of the strain tensor, the volumetric strain.

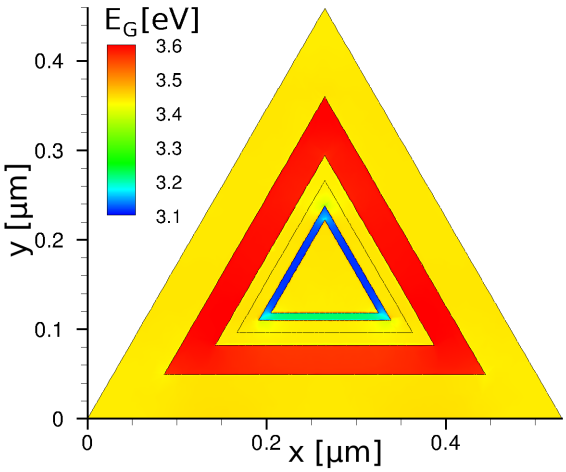


Fig. 3. Strain induced band gap change in a plane parallel to the triangular surface.

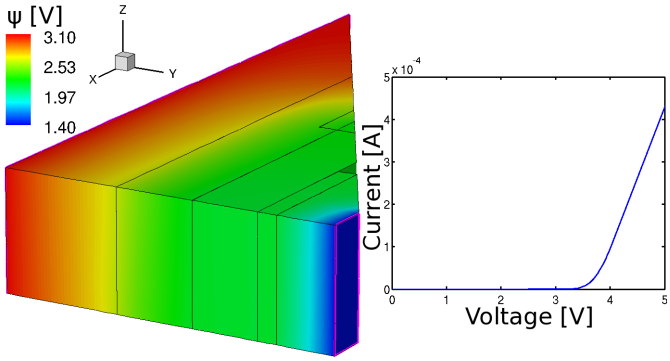


Fig. 4. Potential distribution at 5V bias on a sixth of the structure and U/I curve.

the semipolar QWs have the same sign. This suggests that the latter QWs are not subject to a strong electric field due to piezoelectric polarization. In addition, the semipolar QWs show a higher valence band edge shift but a lower conduction band edge shift than the polar QW resulting in a smaller band gap as shown in Fig. 3.

The numerical modeling of this nanowire LED is challenging as the QW planes are connected in the corners of the triangle and possess different band gaps and polarization fields. In a first simplified approach the transport has been solved with reduced piezo fields for a single quantum well on a sixth of the structure cut along the symmetry edges. The turn on occurs at about 3.5V corresponding to the experimental data. The p-doped region has a relatively high resistivity contributing much to the voltage drop across the device as shown in Fig. 4.

## IV. Outlook

The analysis of strain, strain induced band edge shifts and piezo polarization effects demonstrates that the core/shell nanowire LED has a level of complexity higher that the quantum disk nanowire LED because polar and semipolar QWs are connected in parallel and because of the asymmetric current flow and potential drop over the QWs. The recent analysis has proven that our physics simulator is well suited for these devices. We are working towards a fully coupled and self consistent simulation of the luminescence properties of the core/shell nanowire LED.

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