tdkp/AQUA: Unified Modelling of Electroluminescence in Nanostructures

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Abstract—This article summarizes the capabilities of the optoelectronic simulation framework *tdkp/AQUA* aimed at the description of electroluminescence in semiconductor nanostructures such as light-emitting diodes (LEDs). *tdkp* is a stand-alone finite-element software able to accurately calculate strain, built-in fields due to spontaneous and piezoelectric polarization, quantum states, gain and luminescence spectra in zero- to three-dimensional structures. *AQUA* calculates transport through nanostructures using an original model which accounts for the distinct behaviour of carriers confined to active regions and unconfined carriers. Furthermore, it computes electroluminescence spectra via a self-consistent coupling of the confined carriers to quantum-mechanical calculations using *tdkp*. Two examples are presented which highlight the versatility and generality of the developed simulator.

I. INTRODUCTION

Light-emitting diodes (LED) have become one of the great hopes of the beginning 21st century. Their longevity, superior energy efficiency and impeccable color characteristics destines them as replacements in most lighting applications, giving rise to potential energy savings equivalent to a gigaton of CO_2 per year [1]. In this light it is highly desirable to precisely understand the physical processes governing current devices as well as exploit novel LED concepts.

The simulation framework *tdkp/AQUA* developed by the authors aims at the comprehensive description of the physical processes governing nano-LEDs. In the following Sections, an overview of the employed models is given and two application examples are briefly discussed.

II. MODEL

A. *tdkp - Strain, polarization, quantum states, gain and luminescence*

tdkp [2] is a stand-alone software library based on a continuum description to calculate strain, spontaneous and piezoelectric polarization and its induced potential, quantum states within the multiband **kp** band structure model and gain and luminescence spectra for nanostructures of arbitrary dimensionality. A flexible finite element discretization is employed for all differential equations.

Strain calculations are based on a linear elasticity description. Material interfaces are accurately modeled in calculations of polarizations and induced potentials by the exact inclusion of surface and volume charges.

kp envelope function theory is particularly suitable for optoelectronic structures because it accurately models the band structure around the Γ-point without overextending computational costs. Key to the robustness and reliability of such calculations is the elliptic formulation of the equations [3]. All standard **kp** models for zincblende and wurtzite structures including strain corrections are implemented.

Lastly, gain and luminescence spectra are calculated for a given density using a semiclassical description [4]. Many-body effects such as band gap renormalization can be either neglected (free-carrier level) or treated on the screened Hartree-Fock (RPA) level.

B. *AQUA - Carrier transport and self-consistency with luminescence*

AQUA [5] models carrier transport in a semiclassical picture in which carriers completely lose or retain coherence in a certain direction. The carrier system is partitioned into unbound populations, able to move in all directions, and bound populations confined to the active region, be it a quantum well, wire or dot. Confined carriers are described by their quantum-mechanical wavefunctions in the confinement directions whereas they are able to move by drift in diffusion in the remaining directions.

Coupling of the populations happens through capture, acting as recombination and generation terms in the continuity equations, and the common electrostatic potential. Radiative recombination of bound carriers as well as their shape in the quantized direction(s), influencing the Poisson equation, is calculated using *tdkp*. A predictor-corrector scheme is employed to facilitate self-consistence. Transport equations are discretized using the Scharfetter-Gummel finite volume method and solved by Newton iteration using analytic differentiation with an automated chain rule. So far no temperature or lasing models have been implemented. Furthermore, photon modes for the luminescence are assumed to be free-space and only steady-state situations are considered.
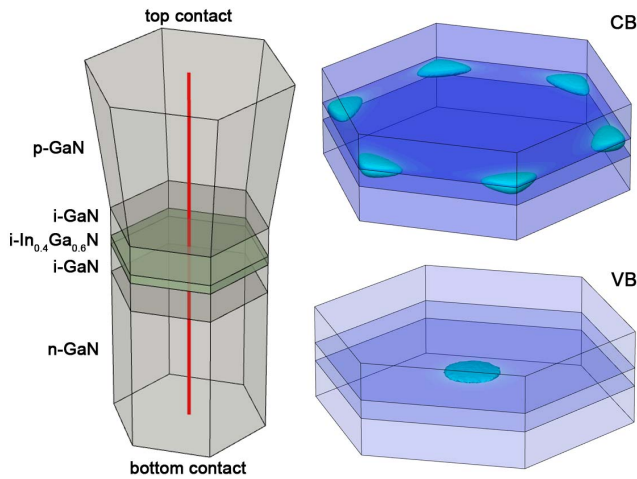
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Fig. 1. Nanocolumn LED structure and first bound 3D electron and hole state including strain and polarization effects.
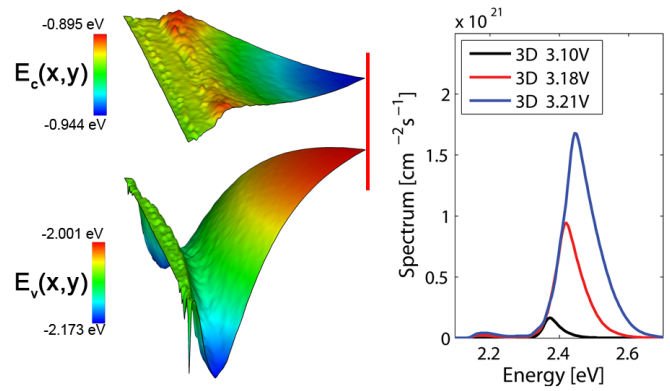

Fig. 2. Nanocolumn LED lateral drift-diffusion potential for bound carriers (only a sixth of the column is shown) and emission spectra.
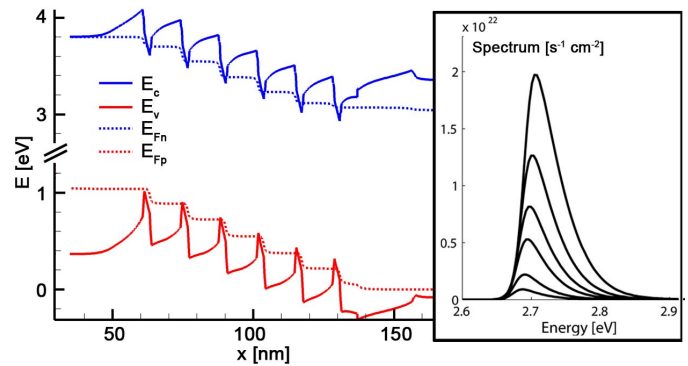

Fig. 3. MQW LED band edges, quasi-Fermilevels and emission spectra near turn-on.

III. APPLICATION EXAMPLES

The InGaN/GaN nanocolumn LED [6], [7] depicted in Fig. 1 has a three-dimensional dependence of many of the quantities mentioned above. A 3D calculation of states bound to the quantum disk shows that when strain and polarization potentials are taken into account, the band edges are rather flat on the inside but drop sharply towards the column surface. Electron states strongly confined in all directions exist near the surface. However, emission is expected to be dominated by states which are extended in lateral direction. Hence a quantum-well picture is adopted where lateral drift-diffusion movement happens in a potential corrected near the surface (Fig. 2). The resulting luminescence mainly stems from the column center where strain approaches the biaxial value.

A second example is the planar InGaN/GaN multi-quantum-well LED shown in Fig. 3 which resembles current high-power commercial LEDs. A central matter in these devices is the efficiency droop at high output power (Fig. 4) which may have several physical origins. Apart from temperature effects, *tdkp/AQUA* is able to describe these mechanisms and provide insight into the importance of electron leakage and Auger recombination.

ACKNOWLEDGMENT

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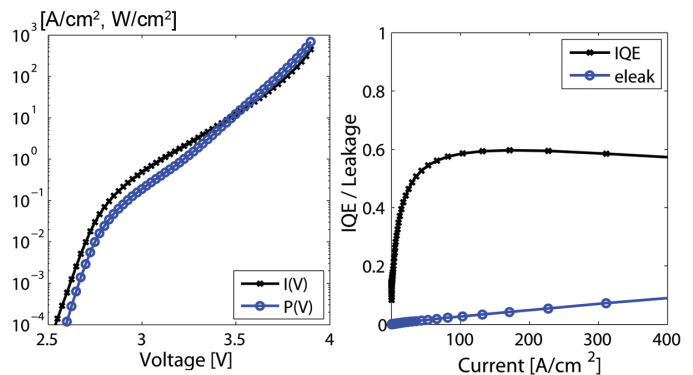

Fig. 4. MQW LED *I-V* and *P-V* curves, internal quantum efficiency and electron leakage.