

# Realistic model of an InGaN quantum-dots active region in a LED structure

Daniele Baretin<sup>1,2</sup>, Matthias Auf der Maur<sup>1</sup>, Alessandro Pecchia<sup>3</sup>, Walter Rodrigues<sup>1</sup>, Andrei F. Tsatsulnikov<sup>4</sup>, Alexei V. Sakharov<sup>4</sup>, Wsevolod V. Lundin<sup>4</sup>, A. E. Nikolaev<sup>4</sup>, Nikolay Cherkashin<sup>5</sup>, Martin J. Hÿtch<sup>5</sup>, Sergey Yu. Karpov<sup>6</sup>, and Aldo di Carlo<sup>1</sup>

<sup>1</sup> Department of Electronic Engineering, University of Rome "Tor Vergata" Via del Politecnico 1, 00133, Rome, Italy

<sup>2</sup> UNICUSANO, Università degli Studi Niccolò Cusano-Telematica Rome, Italy.

<sup>3</sup> CNR-ISMN, via Salaria Km. 29.300, 00017 Monterotondo, Rome, Italy

<sup>4</sup> Ioffe Physico-Technical Institute of the Russian Academy of Science, St. Petersburg, Russia

<sup>5</sup> CEMES, CNRS UPR 8011, Toulouse, France

<sup>6</sup> STR GROUPSOFT-IMPACT, LTD, St. Petersburg, Russia

**Abstract.** Numerical simulations of quantum-dot heterostructures derived from experimental high-resolution transmission electron microscopy results are presented. We analyze a real sample containing large InGaN islands with size of ten of nm and non-uniform In content. The three-dimensional dot models have been directly extrapolated by experimental results. The electromechanical, continuum  $\vec{k} \cdot \vec{p}$ , empirical tight-binding and optical calculations for these realistic structures present very good agreement if compared with experimental evidences, showing that the use of realistic structures can provide significant improvements into the modeling and the understanding of quantum-dot nanostructures.

## Introduction

Recent papers from our group and coauthors have clearly pointed out how taking into account realistic elements possibly derived from experimental evidences can strengthen the effectiveness of models of heterostructure-quantum dots (QDs). As examples in this context we remind the derivation of an average concentration profile obtained using lattice fringe analysis used for simulation of electronic structure of InAs/GaAs QDs [1], extrapolation of a realistic geometry of InP surface quantum dots on a  $\text{In}_{0.48}\text{Ga}_{0.52}\text{P}$  buffer layer used in a finite element (FEM) implementation of 8-band  $\vec{k} \cdot \vec{p}$  model [2], and the study of the impact of inter-dot strain fields on the optical properties of realistic InP quantum-dot molecules [3].

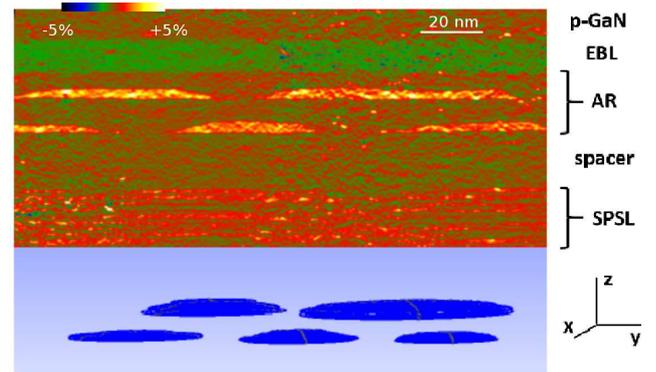
A new possible application of a realistic multi-scale approach is the study of Indium Gallium Nitride systems. In fact, it is well known that an increasing role in the fabrication of LEDs has been played in the last two decades by alloys containing Indium Gallium Nitride (InGaN) [4, 5, 6], since by In content engineering in the active region it is theoretically possible to cover the whole visible spectrum range [7, 8].

Therefore, in this present work we present a realistic model for an LED structure consisting of a thick n-GaN contact layer, a prelayer made of 12 period short-period InGaN/GaN superlattice (SPSL), undoped GaN spacer, active region (AR) including double stacked quantum-dot (QD) layers, p-AlGaN electron blocking layer (EBL), and p-GaN contact layer.

A multiscale approach [9] has been applied to the structures, supporting continuum models based both on the  $\vec{k} \cdot \vec{p}$  [10] with atomistic methods and empirical tight-binding [11, 12, 13] approaches. We mainly focused on the impact of the lateral and vertical coupling of QDs via electromechanical field [14] and of the influence of the inhomogeneity of the In content on the optical properties of the simulated structure.

## 1. Reconstruction of quantum-dot active region

We have developed an appropriate algorithm in order to derive a three-dimensional geometry and structure from the experimental image of the out-of-plane strain obtained by geometric phase analysis (GPA) of the high-resolution transmission electron microscopy (HRTEM) image of a real LED structure [15]. A two-dimensional image of the out-of-plane strain in the structure is shown in the top of Figure 1. By means of the GwyddionTM software [16] we sampled the dots and then extrapolated a three-dimensional structure for the whole active region which is shown on the bottom of Figure 1. The extrapolated structure has been then used



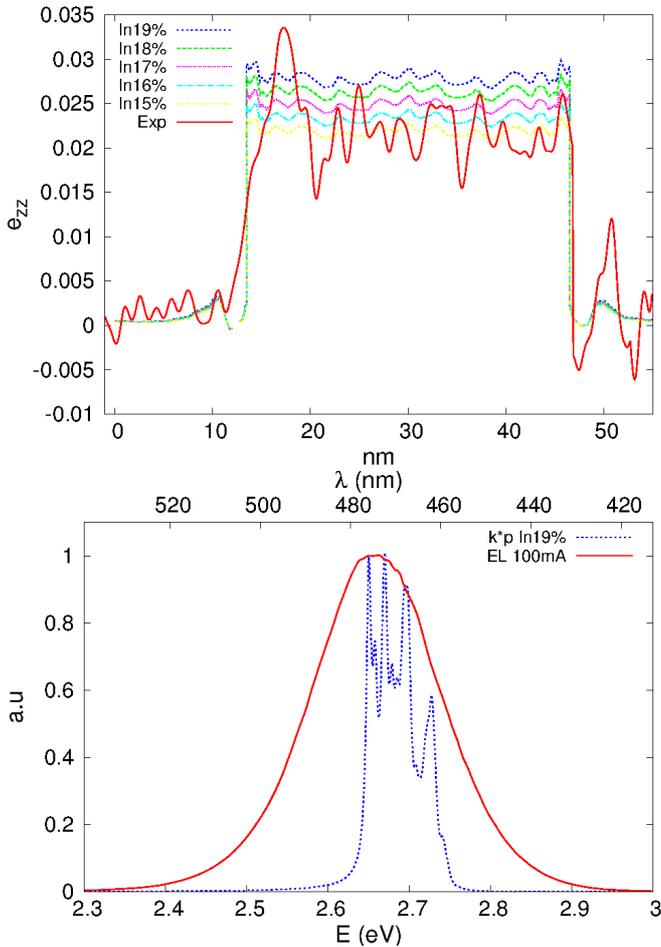
**Fig. 1.** Top: a two-dimensional image of the out-of-plane strain obtained by geometric phase analysis of the HRTEM image used to derive the three-dimensional structure. Bottom: the three-dimensional extrapolated active region structure.

to create a finite element model (FEM) in order to discretize the electro-mechanical, electronic and optical models. Details of the extrapolation method and the numerical models are described in Ref.[2].

## 2. Results

In the top panel of Fig. 2 we compare the experimental strain field  $e_{zz}$  relative to the GaN substrate along the  $y$ -axis (perpendicular to growth direction) with the continuum

model results assuming different In content in the single QD approximately located in the center of the sample, a comparison which gave us a good insight into the real average InGa<sub>0.81</sub>N composition of the dots. From this comparison, the In content was estimated to be approximately 19%. The plot in the bottom panel compares the experimental electroluminescence (EL) spectrum of the whole LED structure and the  $\vec{k} \cdot \vec{p}$  emission spectrum of the central quantum dot (In 19%). The comparison demonstrates very good agreement between theoretical and experimental peak photon energies, whereas the spectra widths are different. A superimposition of the experimental EL and  $\vec{k} \cdot \vec{p}$  spectra calculated for all the dots in the active region (not shown here) provides an almost coincident overlap between the calculations and measurements, ensuring the validity of our model.

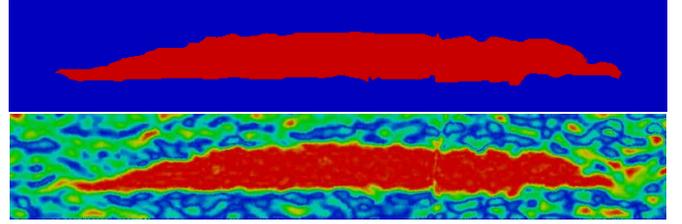


**Fig. 2.** Experimental out-of-plane strain along the y-axis compared with numerical results obtained for different In content (%) (top) and the experimental EL spectrum compared with numerical  $\vec{k} \cdot \vec{p}$  spectrum of an individual QD (bottom).

We also will present results showing the impact of lateral and vertical electromechanical coupling between the dots on the optical properties of the LED structure by means of a full three-dimensional model of the sample.

Furthermore, a qualitative analysis of the impact of local In content on the optical properties using different two-dimensional models has been carried out. The case of a uniform averaged distribution (In 19%) with a realistic structure has been compared with a real local distribution given by experimental data implemented with an *ad hoc* algo-

rithm. In Figure 3, these two FEM structures are compared. Recommendations on the choice of the structural model optimal for simulations are given on the basis of the comparison.



**Fig. 3.** Top: QD structure with a uniform In distribution (19%). Bottom: the structure derived by an algorithm which reads the real local In content and creates the correspondent structure.

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