

Realistic model of LED structure with InGaN quantum-dots active region

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

I. INTRODUCTION

In recent papers from our group and coauthors have clearly pointed out how taking into account realistic elements directly derived from experimental results can strengthen the effectiveness of models of an heterostructure-quantum dot (QD). The derivation of an average concentration profile obtained using lattice fringe analysis used for electronic calculations of InAs/GaAs QDs [1], the 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], these are all recent interesting examples of application of a realistic model with numerical results very close to experimental reality.

Nowadays, a new possible field of application of a comprehensive realistic multiscale [9] approach appears to be the analysis of Indium Gallium Nitride systems, because of the increasing role in the fabrication of LEDs the alloys containing Indium Gallium Nitride (InGaN) have been playing in the last two decades [4]–[6], whereas it is theoretically possible to cover the whole visible spectrum range by engineering the In content in the active region [7], [8].

Therefore, we present realistic model of 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. Both continuum models as the $\vec{k} \cdot \vec{p}$ [10] and atomistic methods, as the empirical tight-binding [11]–[13] have been combined within a multiscale approach.

We studied the impact of the lateral and vertical coupling via electromechanical field [14], the influence of the inhomogeneity of the In content on the optical properties of the sample and we also show as simulations result can be used for the optimization of current injection in quantum-dot device.

II. STRUCTURES FOR QUANTUM-DOTS

A complex algorithm has been developed in order to build a three-dimensional geometry and a 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 sample [15]. The latter contains several InGaN/GaN superlattices and large InGaN QD islands having sizes of tens of nanometers, with non-uniform In distribution. A two-dimensional image of the out-of-plane strain in this sample is shown in the top of Figure 1.

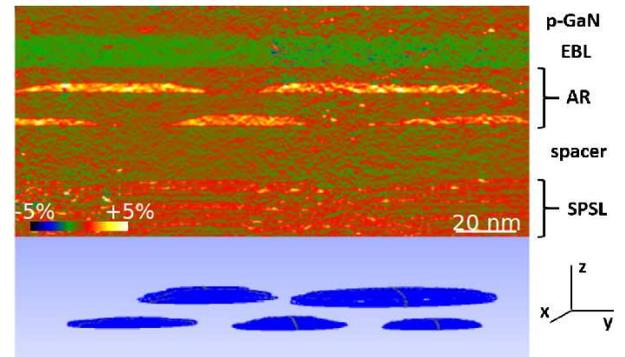


Fig. 1: Top: The two-dimensional image of the out-of-plane strain obtained by geometric phase analysis of the HRTEM image used to derive the three-dimensional structure. Bottom: the three-dimensional extrapolated structure.

Using the GwyddionTM software [16] we sampled the QDs and extrapolated a three-dimensional structure for all the sample, showed on the bottom of Figure 1. The details of the extrapolation method and the numerical models are described in Reference [2]. This extrapolated structure has been used to create a finite element model (FEM) to discretize the electro-mechanical, electronic and optical models.

III. RESULTS

We compare the experimentally measured strain field e_{zz} relative to the GaN substrate along y axes (perpendicular to growth direction) with continuum model results assuming different In % for the single quantum dot approximately located in the center of the sample (top panel of Fig. 2). This comparison is very useful, since it provide us an insight about the actual average content of the dots we have used for the bandstructure calculations, which we estimated to be approximately 19%. Thus the plot in the bottom panel shows a comparison between the Electroluminescence (EL) of all the sample and the $\vec{k} \cdot \vec{p}$ spectrum of the central quantum dot with a 19% Indium content. It is important to notice that this simulation does not consider the larger QDs, so the dots with lower-energy spectrum, but still the agreement is very good in the peak photon energy. The superimposition of the spectra calculated for all the dots of the sample with the experimental EL (not showed here) presents an almost coincident overlap between simulations and measurements, ensuring the validity of our model.

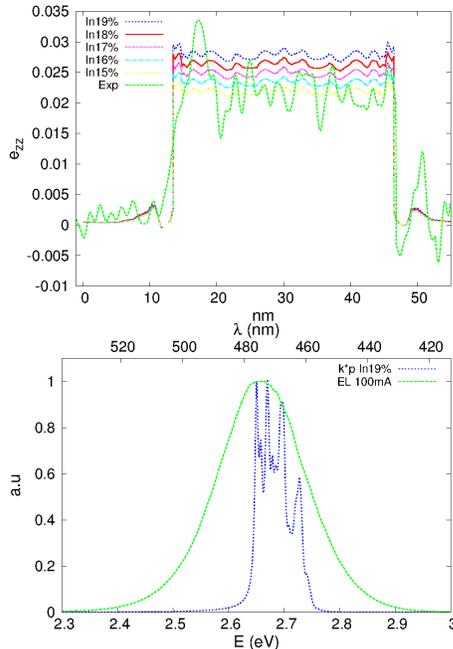


Fig. 2: Experimental out-of-plane strain profile along y axis compared with numerical results with different In content (%) (top) and the experimental EL spectrum compared with numerical $\vec{k} \cdot \vec{p}$ spectrum with 19% of In content (bottom).

We will present results concerning the impact of lateral and vertical coupling between the dots on the optical properties of

the sample analyzing effects due to inter-dot electromechanical fields, using a complete three-dimensional simulation of the sample.

Furthermore, it will be shown a qualitative analysis also of the impact of local In content on the optical properties using different two-dimensional, since a case of a uniform averaged distribution (In 19%) with a realistic structure has been compared with a real floating local distribution given by experimental data implemented with an *ad hoc* algorithm. The two correspondent FEM structures are showed in Figure 3.

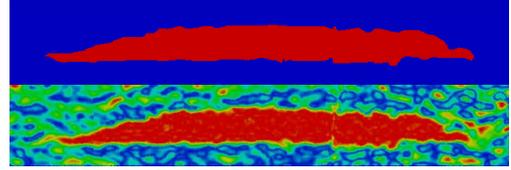


Fig. 3: Top: the structure with an uniform In distribution (19%). Bottom: the structure derived by an algorithm which reads the real local In content (Color map proportional to composition distributions).

The realistic model of LED structure with QD active region built up in a way described above enables simulation of the electron and hole transport which is found to differ remarkably from that occurring in the structures with uniform quantum wells.

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