Realistic models of quantum-dot heterostructures

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***Abstract*—Different numerical simulations of quantum-dot heterostructures derived from experimental results are presented. We extrapolated three-dimensional dot models directly by atomic force microscopy and high-resolution transmission electron microscopy results, and we present electromechanical, continuum $\vec{k} \cdot \vec{p}$, atomistic Tight Binding and optical calculations for these realistic structures, also compared with benchmark calculations with ideal structures largely applied in the literature. According our results, the use of more realistic structures can provide significant improvements into the modeling and the understanding of quantum-dot nanostructures.**

I. Introduction

It is fairly well established that taking into account realistic elements possibly derived from experimental evidences can enhance the effectiveness of a model of an heterostructures quantum dot (QD). In this context with some coauthors we have recently presented models where either a realistic concentration profile or a realistic shape and geometry were implemented. In the former by the extrapolation of an average concentration profile using lattice fringe analysis some electronic calculations of InAs/GaAs QDs have been presented [1], in the latter the shape and the geometry of InP surface quantum dot have been directly extrapolated by experimental two-dimensional atomic force microscopy results [2]. This structure has been used for a finite element (FEM) implementation of 8-band $\vec{k} \cdot \vec{p}$ model [3], including electromechanical fields [4], which has showed significant differences compared with previous results in literature, indicating the need for taking into account not only the real dot shape and geometry, but inter-dot effects as well, as for instance inter-dot strain fields.

Following on from these results, here we present some realistic models of quantum dots derived from different experimental samples with differences techniques. Besides, we apply a multi-physics approach to the structures, supporting continuum models as the $\vec{k} \cdot \vec{p}$ with atomistic methods, as the empirical tight-binding [5]–[7].

II. Structures and Models

A first set of realistic structures we implemented regards InP surface quantum grown epitaxially on $In_{0.48}Ga_{0.52}P$ buffer layer lattice matched to a Si doped GaAs substrate [8]–[11].

We have singled out a quantum dot from the atomic force microscopy (AFM) of an homogeneous sample, which is showed on the left side of Figure 1. By GwyddyonTM software [12] we sampled the dot extrapolating a three-dimensional structure, which is shown on the right side of Figure 1.

The extrapolated structure has been used to create a finite element model (FEM), used to discretize the electromechanical, electronic and optical models. We remand to Ref. [2] for a complete description of the extrapolation method and the numerical models.

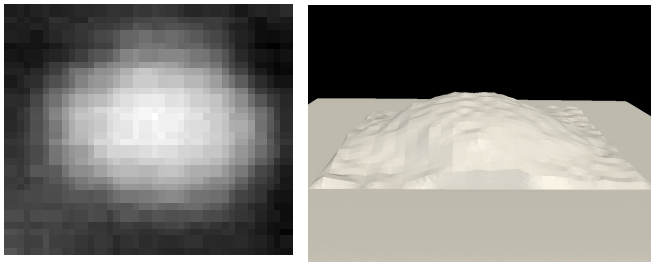

Fig. 1: Left: 2D AFM micrography of the specific QD we used in our calculations. Right: 3D extrapolated structure.

We have developed an analogous algorithm to derive a three-dimensional geometry and structure from high-resolution transmission electron microscopy (HRTEM) images of a more complex sample, whih contained InGaN/GaN superlattices together with large InGaN QD islands having sizes of tens of nanometers, having the QDs a non-uniform In distribution.

In Figure 2 we show a two-dimensional image of an InGaN QD elaborated by Gwyddion software from HRTEM results, which has been used to implement a three-dimensional structure.

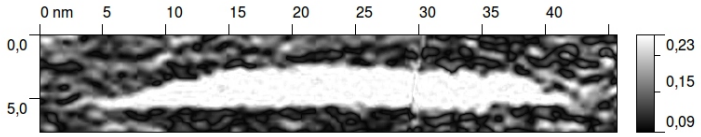

Fig. 2: A 2D image of an InGaN QD elaborated by Gwyddion software from HRTEM results. The gray scale indicates the In content.

Interestingly, the numerical results of the strain fields which we can calculate with our model can help to determine more accurately the fluctuations of Indium initially measured with experimental techniques.

III. Results

The results from calculations using realistic shape and geometry directly derived from experiments have often showed remarkable difference with results of ideal models with symmetrical geometries given by analytical expressions, which were usually presented in the previous literature. In contrast, we found reasonable and better agreements with measured

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quantities, as for example, experimental photoluminescence (PL) spectra and optical spectra given by our simulations.

This gave us new insights for the understanding of the properties of these structures. In the case of the InP surface QDs, for instance, some differences between the numerical and the PL spectrum seemed to indicate a lack of photoluminescence response from the smaller dots contained in an homogeneous sample with a high density of dots [2], hypothesis which has been a posteriori confirmed by further experimental measurements.

Our analysis demonstrates that the lack of PL response from these small dots could be due to strong inter-dot strain fields, supporting a conjecture that a realistic simulation could include some inter-dot effects, namely a simulation of coplanar quantum-dot molecules.

This can be observed in Figure 3, where a plot of the absolute value of strain fields for an InP/$In_{0.48}Ga_{0.52}P$ QD molecule is showed.

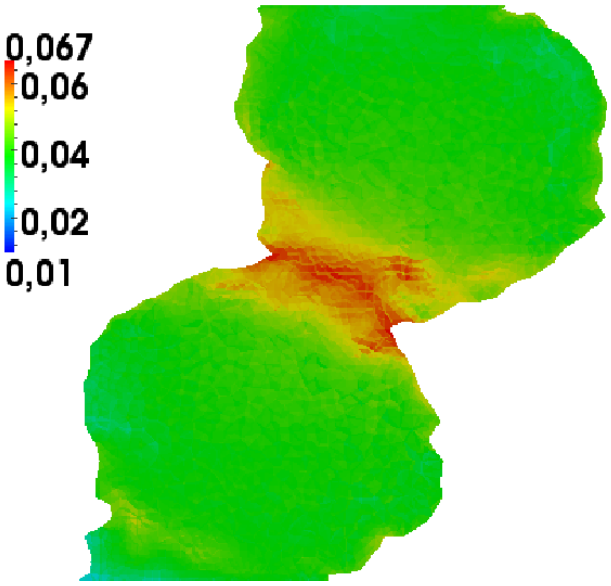

Fig. 3: The magnitude of the absolute value of strain fields for a coplanar QD molecule.

The strong strain fields we can see in the junction area between the two QDs can remarkably modify the confinement potential of the two structures, and consequently affect the numerical optical spectrum. This can explain the experimental PL data, that is the lack of PL response from the smaller dots of a dense sample.

We present a similar analysis in the case of the complex sample including the InGaN QD. A more accurate understanding of the optical properties of this system could be helpful in the realization of new devices based on inorganic light light-emitting diodes (LEDs), since a relevant role in the fabrication of LEDs will be soon played by Indium Gallium Nitride alloys [13]–[15].

Finally, from a speculative point of view, our results could give an answer to the long debate on the accuracy of the continuous $\vec{k} \cdot \vec{p}$ approach as compared with atomistic models. Our atomistic calculations, which follow a multi-physics paradigm approach for the modeling of structures and devices [16], may definitively clarify some of the issues of this unresolved debate [17]–[19].

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