Electronic and transport properties of GaN/AlGaN quantum dot-based p-i-n diodes

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Abstract—**Quantum dot (QD) systems based on III-nitride have recently shown to be very promising nanostructures for high-quality light emitters. In this work, electronic and transport properties of AlN/GaN QDs are investigated by means of the TiberCAD software tool, which allows both a macroscopic and an atomistic approach, with the final aim to couple them in a multiscale simulation environment.**

I. Introduction

Recent interest in III-nitride quantum dot (QD) systems is due to their high potential as high-quality light emitters in the visible to ultraviolet spectral range [1]. AlN/GaN QDs are indeed promising structures for variable-wavelength devices since they possess a high luminescence efficiency. In fact, due to a large band discontinuity in the GaN/AlGaN heterostructure, self-assembled QDs based on these materials seem to be ideal candidates for tunable room-temperature light-emitting devices.

In this work we use our TiberCAD software tool [2] to study the properties of a AlGaN/GaN QD in a AlGaN nanocolumn p-i-n diode structure.

The TiberCAD project is aimed at the implementation of a device simulation tool which on the one hand satisfies the need for a multiscale simulation environment and on the other hand handles the most important physical issues that the present and the next electronic and optoelectronic devices have to face. Some of these are strain and strain-induced effects, self-heating / thermal transport, transport of electrons, holes and of other quasi-particles as excitons/polaritons, quantum mechanical effects such as confinement and tunneling and quantum mechanical transport.

In particular, on the one hand the down-scaling of device dimensions, driven by the need for high performance devices and high integration, requires the inclusion of advanced quantum mechanical models beyond classical transport theories. On the other hand, usually the active region of a device which needs a more elaborate and careful treatment is small compared to the overall simulation domain.

The computational cost of the more accurate model can prevent its application to the whole device. A possible solution to these issues is a multiscale simulation software, capable to implement different models at different length scales, ranging from macroscopic to atomistic representations. Depending on the case, it implements the more computational demanding approaches only when necessary and relies on approximated, but faster methods otherwise.

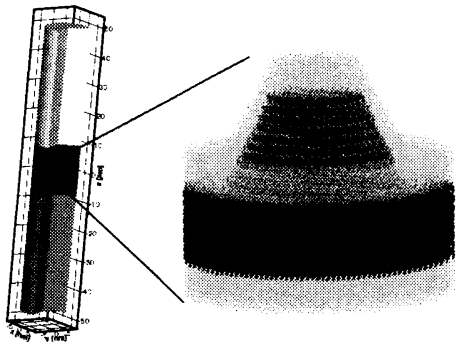

Fig. 1. Model structure of the AlGaN/GaN quantum dot system.

For example, in nanostructure-based devices such as quantum-dot LEDs, methods based on the envelope function approximation (EFA) – widely used for the description of heterostructures – can break down and atomistic approaches become inevitable [3]. Due to their high computational cost, however, atomistic models are limited to rather small structures consisting of up to ten-thousands of atoms. A reliable simulation of a device including not only the nanometric active regions, but also the substrate and contact regions has therefore to be done by coupling atomistic approaches to semi-classical models in the framework of a multiscale simulation.

II. Theoretical Models

The calculations have been performed with the multi-scale software tool TiberCAD [2]. The physical models implemented in TiberCAD are described in the following.

The calculation of strain in lattice mismatched heterostructures is based on linear elasticity theory of solids, assuming pseudomorphic interfaces between different materials [4]. As a result we obtain the strain tensor in any point of the structure, the shape deformation and the piezoelectric polarization.

The particle flux is written in terms of driving forces represented by the electro-chemical potential and temperature gradients, i.e. $j_i = \mu\rho(\partial_i\phi + P\partial_i T)$, where μ is the mobility, ρ is particle density and P is the Seebeck coefficient. The particle continuity equations are solved self-consistently with the Poisson equation, which includes spontaneous and piezoelectric polarization.

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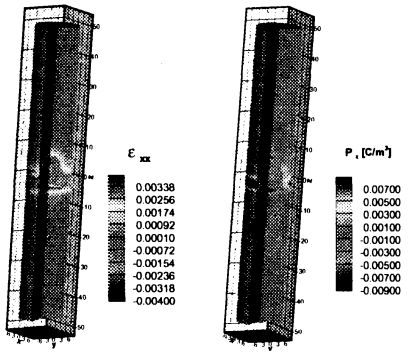

Fig. 2. ε_{xx} strain component (left) and z-component of the piezoelectric polarization (right).

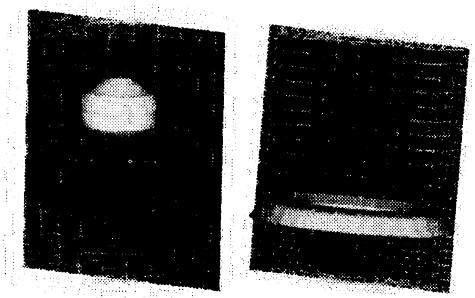

Fig. 3. First confined electron (left) and hole (right) states

Self-heating effects are calculated by means of a macroscopic thermal simulation. The Peltier-Thomson effect is also included.

The calculation of the eigenstates of confined particles is based on the envelope function approximation (EFA) including single-band and multiband $\mathbf{k}\cdot\mathbf{p}$ approaches. From the stationary Schrödinger equation we obtain energy spectrum, particle density, probabilities of optical transitions and emission optical spectra [5]. Semiconductor band parameters used for the semiclassical transport calculations are obtained from a bulk $\mathbf{k}\cdot\mathbf{p}$ calculus including corrections due to strain [6].

III. Results

A model structure of a $Al_{0.3}Ga_{0.7}N$ nanocolumn surrounding a 5 nm-size conical GaN quantum dot has been constructed (see Fig.1); the two ends of the nanocolumn are doped with a concentration $10^{19}cm^{-3}$ respectively p-type and n-type, while the quantum dot region is intrinsic. Based on the geometric information, an atomistic model of the quantum dot (also shown in Fig.1) can be generated and used to perform full-band empirical tight-binding calculations.

First, strain map has been calculated with the model present in TiberCAD . In Fig.2 the ε_{xx} strain component is reported. Since GaN lattice constant is lower than for $Al_{0.3}GaN$, the quantum dot is subjected to a compressive strain in the planar directions, so that the ε_{xx} component has a negative sign inside the GaN quantum dot and is positive outside. On the contrary, ε_{yy} strain component is positive inside the dot and

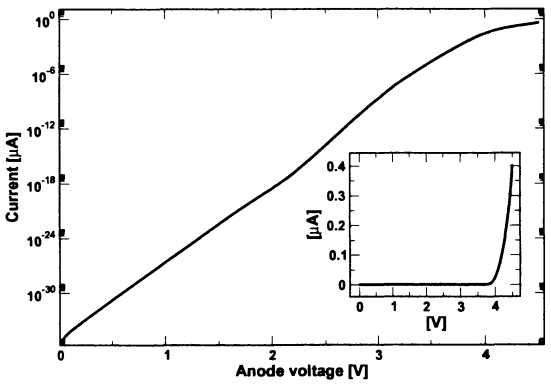

Fig. 4. IV characteristic of the nanocolumn diode

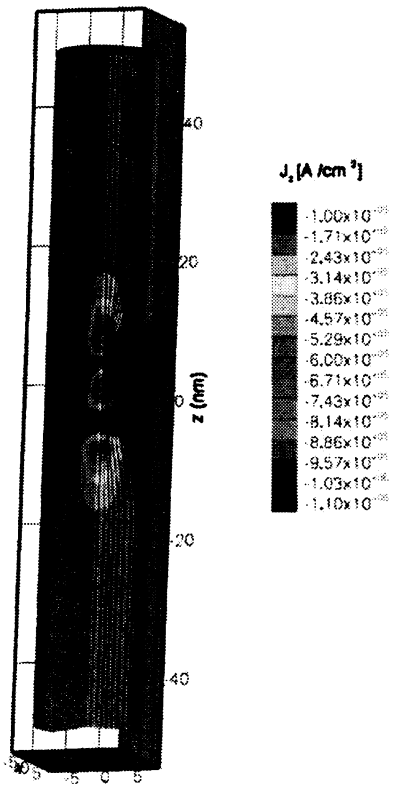

Fig. 5. Current density in the nanocolumn diode

negative outside, vanishing in the AlGaN bulk; this is due to the fact that AlGaN material is taken as the substrate reference material.

The strain results indicate a generally inhomogeneous strain map. As a consequence, also the piezoelectric polarization induced by strain, shown in Fig.2 (at right) is inhomogeneous, even if it is mostly localized around the GaN quantum dot. The piezoelectric polarization, together with the spontaneous polarization, are crucial to determine the band profile of the

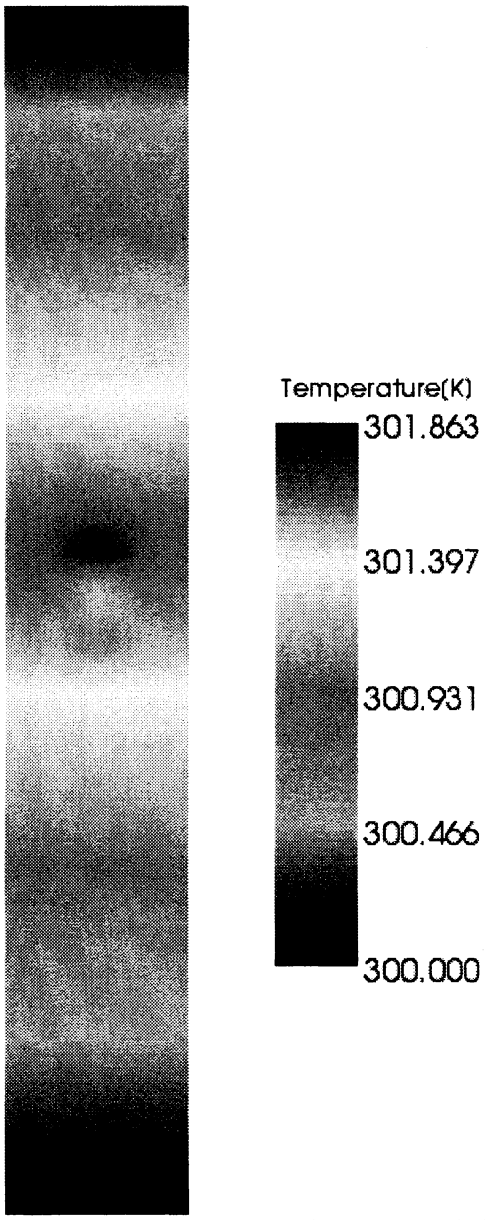

Fig. 6. Temperature map in the nanocolumn diode

heterostructure and thus the confinement of the quantum dot.

Quantum-mechanical models based on the envelope function approximation (EFA) are used to solve Schrödinger equation and to obtain the eigenstates in the QD and the particle quantum density; a single-band model for conduction band and a multiband 6x6 $\mathbf{k} \cdot \mathbf{p}$ model for valence band are applied. In Fig.3 the first confined eigenstate in the quantum dot at the equilibrium is shown, respectively for electrons and holes.

A transport model in a semi-classical framework, based on drift-diffusion approach is applied to calculate current in the nanocolumn p-i-n diode, when a bias is applied between the two contacts; the obtained IV characteristic is shown in Fig.4.

In Fig.5 we show the component of the total current density along the growth direction. It can be seen that the current

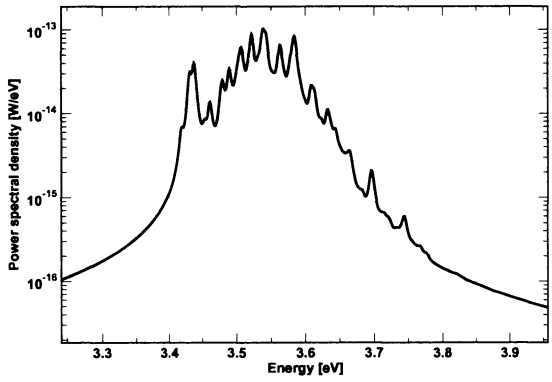

Fig. 7. Optical emission spectrum for V = 3.7V

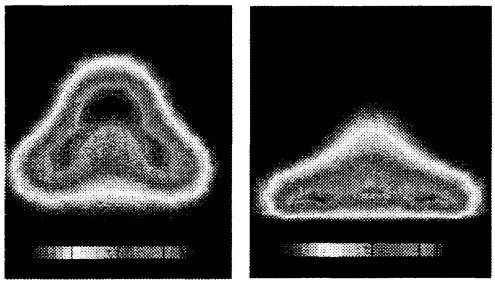

Fig. 8. Quantum electron (left) and hole (right) densities in the dot

flow is confined in the QD region. This effect leads to higher Joule's effect in such region and, therefore, more heating (see the temperature map in Fig. 6).

From the optical $\mathbf{k} \cdot \mathbf{p}$ matrix elements, the emission optical spectrum for $\mathbf{k}$=0 is calculated. Fig.7 shows the calculated emission spectrum for a bias of Vd = 3.7V, just above the threshold voltage, corresponding to a current of $5 \times 10^{-4} \mu A$.

Finally, the quantum electron and hole densities are calculated with the EFA models described before, for a bias of Vd = 4V, well above the threshold voltage, corresponding to a current of 0.02 μA. As can be seen in Fig.8, the results clearly show the effect of the confinement of the charge in the QD region.

IV. Conclusion

In this work, we have studied the electronic and transport properties of a p-i-n diode embedding a GaN/AlGaN quantum dot. Results have been obtained with the multiscale software tool TiberCAD , which allows to perform several calculations from different physical models in an integrated code. Thus, strain maps results are used to calculate polarization charge and current in the pin diode. Confinement of the current through the dot is clearly shown, as well as of the quantum charge density and of the quantum states for conduction and valence band. The optical emission spectrum is also shown.

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