Atomistic simulation of InGaN/GaN quantum disk LEDs

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Abstract-In this work we investigate electronic and optoelectronics properties of InGaN/GaN nanocolumn quantum disk LEDs. Calculations have been performed with an atomistic tight-binding model. Results show that emission energies have a minor dependence on the nanocolumn dimension.

INTRODUCTION

In the last years, nanocolumn structures have been designed to realize GaN based light emitting structures. Taking advantage of defect-free nanorods, it is possible to obtain nanostructured InGaN emitters which should lead to very high efficiencies and the possibility to cover the full visible spectrum.

In this work we use the multi-scale software tool TiberCAD [1] to study the electronic and optical properties of a GaN nanocolumn p-i-n diode structure with an InGaN quantum disk (QD). Calculations are performed for several values of column width and In concentration, with an atomistic approach based on empirical tight binding (ETB).

METHODS

Quantum mechanical approaches used in the simulation of nanostructure devices can be based on a continuous media model, or they can exploit the atomistic nature of the device. A widely used method for studying semiconductor heterostructures is the envelope function approximation (EFA). Being a continuous media model, approaches based on EFA eventually break down for very small structures and an atomistic description becomes inevitable. An efficient atomistic approach is that based on the empirical tight binding (ETB) method. In this method the electronic states are written as a linear combination of atomic orbitals (LCAO)[2]. TiberCAD is a software package which provides an integrated multiscale and multiphysics simulation environment capable of coupling physical models at continuous media scale, such as EFA, strain and drift-diffusion and at atomistic scale, like ETB. The atomistic structure, which is needed for ETB calculations, is generated internally in TiberCAD according to the macroscopic device description and crystallographic orientation.

The generation algorithm allows for pseudomorphic heterostructures and it is able to deform the atomistic structure according to the strain obtained from the continuous media elasticity model by projecting the deformation field onto the atomic positions. In a similar way, the macroscopic electrostatic potential calculated with the Poisson/drift-diffusion model is projected onto the atomic positions in order to couple the atomistic calculation of electronic states with the continuous media model for particle transport.

The solution of the eigenvalue problems resulting from the EFA and ETB models provides the energy spectrum, the particle densities and the probabilities of optical transitions. The particle densities can be fed back to the Poisson/drift-diffusion model for self-consistent Schrödinger-Poisson/drift-diffusion calculations. In the case of ETB, the resulting density has to be projected onto the finite element mesh used for the continuous media models. This projection is done using an exponentially decaying function centered on each atomic site. As particle transport is still described in the drift-diffusion approximation, the consideration of quantum mechanical particle densities can be seen as a quantum correction to the local density of states.

RESULTS

A model structure of a GaN nanocolumn with an embedded 2 nm-thick InGaN quantum disk (QD) has been designed (see Fig. 1). The nanocolumn is around 1 μm high and has an hexagonal base with a radius varying between 6.8 and 10.2 nm. A p-i-n diode structure is realized by assigning doping to the contact regions with a donor concentration of 1.5×10^{18} cm^{-3} for the n-doped region and 5×10^{17} cm^{-3} for the p-doped region (190 nm-high), while the InGaN QD region is kept intrinsic. Calculations have been performed for 10% and 20% of In concentration in the InGaN QD. The generated atomistic structures contain from 73000 to 160000 atoms. We have applied a bias of 3.4 V, then we have calculated the eigenstates and eigenfunctions of the system with a TB model based on a $sp^3d^5s^*$ parameterization. The macroscopic electrostatic potential which is projected on the atomic positions is determined by the self-consistent electric field due to doping and polarization.

In Fig. 2 we show the calculated first hole (yellow) and electron (green) quantum states for the column with a radius of 6.8 nm and 10% In concentration.
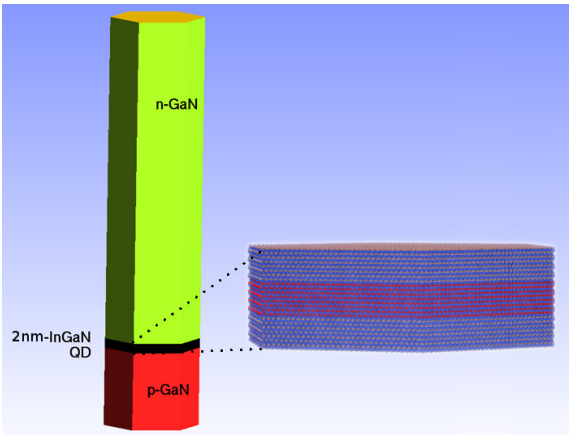
Fig.1 Model structure of the nanocolumn

The spatial separation of electron and hole states is the effect of the polarization-induced electric field.
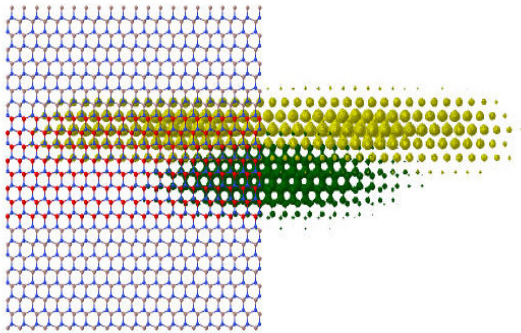

Fig.2 Conduction (green) and valence (yellow) band ETB states in a $In_{0.1}GaN$ QD with a radius of 6.8 nm.

In Fig. 3 we show the dependence of emission energy, obtained from the fundamental transition, on the nanocolumn radius, for In concentration of 10 and 20%.

It can be seen that for 10% In the emission energy increases by 15 meV when column radius decreases form 10.2 to 6.8 nm. For higher In concentration, emission energy tends to increase slightly more. For a fixed column width, emission energy reduces by about 240 meV from 10 to 20% In concentration, due to the lower energy gap and a higher polarization field in the QD.
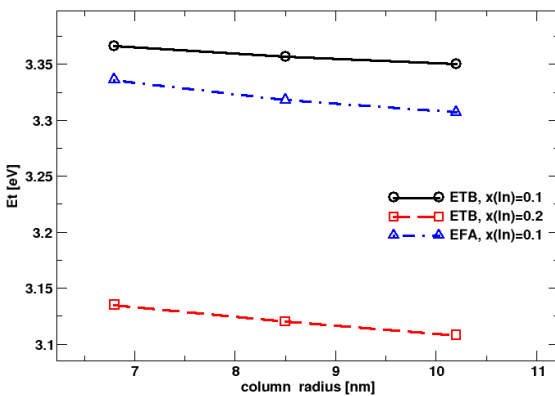

Fig.3 Emission energies for several column radii and In concentrations
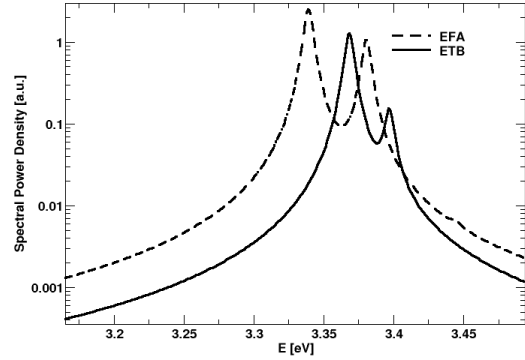

Fig.4 Optical emission spectra for a $In_{0.1}GaN$ QD with a radius of 6.8 nm: results for ETB and EFA models.

We calculated quantum states for the same structures with a 6 bands EFA k·p model, for x(In) =0.1. Fig. 3 shows that the EFA results are underestimated by around 35 meV with respect to full-band ETB calculations. Eigenstates are used to calculate the optical emission spectrum. In Fig. 4 the spectrum obtained for a $In_{0.1}GaN$ QD with a radius of 6.8 nm with ETB is compared with the EFA model.

CONCLUSIONS

We can conclude that the variation of geometrical parameters has a minor effect on QD emission energies, at least for the here examined range.
Moreover, for small values of QD thickness and column width, the results of atomistic tight-binding calculations differ from those of EFA, as the latter lacks a full-band description and does not include the effects at the material interfaces.

ACKNOWLEDGMENT

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