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Enhanced semiclassical simulation of InGaN/GaN multi-quantum-well solar cells

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***Abstract*—This work presents an investigation on a multi-quantum-well InGaN/GaN solar cell, based on our in-house quantum-corrected drift-diffusion simulator D1ANA. Having validated our approach with a commercial simulation tool, it is now ready to provide deep insight into the carrier transport dynamics occurring in these devices, allowing comparisons with experimental results performed under different illumination conditions.**

I. Introduction

III-nitride semiconductors are ideal candidates for next-generation photovoltaics. In fact, InGaN alloys can cover the entire solar spectrum thanks to their continuous bandgap coverage spanning from 0.64 to $3.4\,\mathrm{eV}$, with very high absorption coefficient [1], [2]. Moreover, the unique thermal stability enables operation at $> 400\,^{\circ}\mathrm{C}$ temperatures, and consequently their employment in space missions near the Sun [3]. Increasing the indium content in the alloy extends the absorption range, but the large lattice mismatch between InN and GaN prevents from achieving high crystalline quality InGaN layers. The solution to this problem is to build multi-quantum-well (MQW) solar cells, exploiting the biaxial stress to keep the growth coherent, allowing for higher indium content than in thick layers.

In this work we present an exploratory study of the solar cells described in [4] and sketched in Fig. 1. The device is grown on a sapphire substrate. Its active region, which consists of 25 pairs of $\mathrm{In_{0.15}Ga_{0.85}N}$/GaN QWs ($2.2\,\mathrm{nm}$ wells, $4.8\,\mathrm{nm}$ barriers), is sandwiched between an n-type GaN buffer layer with donor doping density $N_\mathrm{D} = 5 \times 10^{18}\,\mathrm{cm}^{-3}$ and a p-doped GaN layer with acceptor doping density $N_\mathrm{D} = 5 \times 10^{17}\,\mathrm{cm}^{-3}$. The top contact includes Ni/Au grids, placed on a current spreading layer.

II. Results and outlooks

The uniform carrier injection on the device transverse section is guaranteed by the current spreading layer, justifying the choice to reduce the analysis to a longitudinal, 1D problem. The simulations have been performed with our in-house carrier transport simulator D1ANA. This code, which has been already applied to the simulation of VCSELs [5], [6] and solar cells [7], [8], solves the Poisson's equation

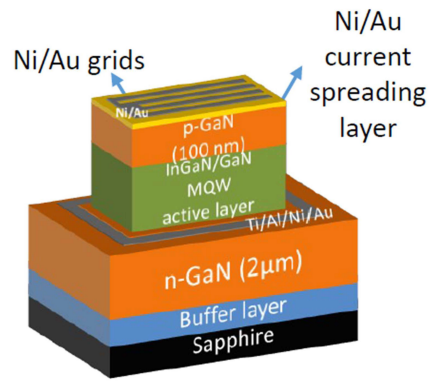

Fig. 1. Geometry of the multi-quantum-well solar cell under investigation.

coupled selfconsistently with the electron and hole continuity equations. The differential equations are discretized by means of a finite difference scheme, where the inherent instability of the drift-diffusion constitutive relations has been treated by the Scharfetter and Gummel formulation [9], [10]. High carrier densities are properly described by Fermi-Dirac statistics, and the incomplete ionization of the doping concentrations is accounted for, which is fundamental for p-type GaN layers.

Figure 2 shows the band diagram of the structure in dark, short circuit conditions. The impact of spontaneous and piezoelectric polarization effects, which are included as sheet charges at the InGaN/GaN heterointerfaces, can be noticed at a glance by recognizing the peculiar potential profile in the QWs. In these simulations, the sheet charges are screened to the 42% of the value predicted by Bernardini and Fiorentini [11], [12].

The two groups of curves have been obtained with D1ANA (solid blue) and with Synopsys Sentaurus Device (dashed red) [13] to perform a cross-validation of the in-house and commercial approaches. Towards a more rigorous treatment of the active region, but less computationally intensive than genuine quantum models [14], [15] or high-order semiclassical pictures [16], [17], D1ANA have been enhanced with *quantum corrections*, which provide a better picture of the interaction between the extended current-carrying states with the localized

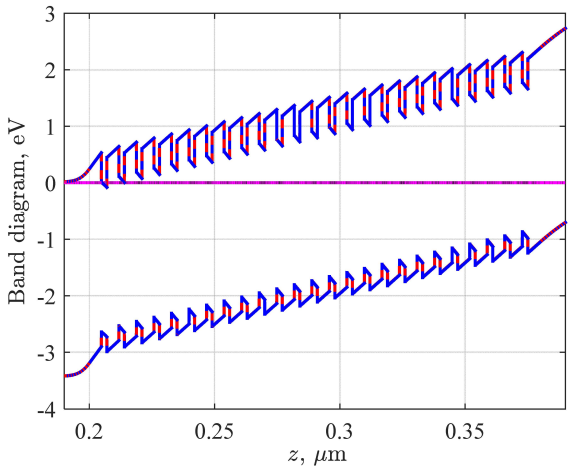

Fig. 2. Band diagrams of the solar cell simulated at dark, short circuit conditions. The solid blue and dashed red curves are obtained with D1ANA and Synopsys Sentaurus Device.

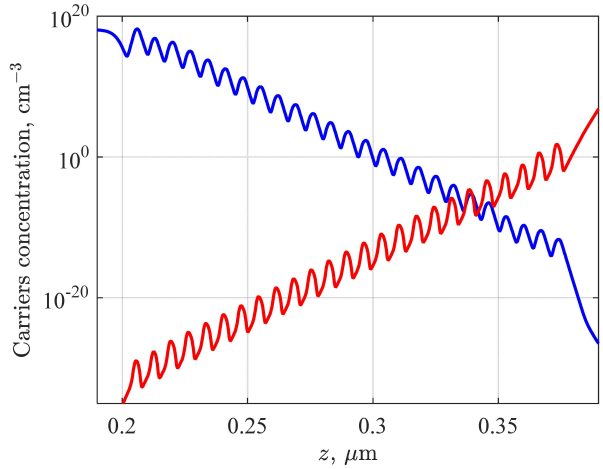

Fig. 3. Electron (blue curve) and hole (red curve) concentrations simulated at dark, short circuit conditions. The simulations have been performed with D1ANA, including the quantum corrections.

states of the nanostructures, involved in the optical emission processes.

These corrections are realized by separating carriers into two sub-populations: bulk carriers, whose transport can be described by standard drift-diffusion, and bound carriers, whose motion is inhibited along the QW confinement direction [14], [18]. The two populations are coupled through a capture term [14], [18], [19], [20], [21], whose impact is controlled by a capture time describing phenomenologically the scattering rate [22]. As a preliminary result, Fig. 3 shows the electron and hole densities obtained with the quantum-corrected drift diffusion. The QW charges are distributed according to their envelope wavefunctions, as it could be appreciated by the smooth charge decays in the barriers. Such wavefunctions are computed by solving Schrödinger's equation selfconsistently with the potential profile obtained from Poisson's equation. Quantum-confined Stark effect is then included, even if it has a minor impact on the recombination processes being the QWs quite narrow.

Having assessed these models, it is now possible to apply them to comparisons with the results of the experimental characterizations performed at Università di Padova under illumination conditions, with the aim of explaining the carrier transport dynamics occurring in these structures.

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