Transport modeling of InGaN/GaN multiple quantum well solar cells

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Introduction

InGaN alloys have been extensively used to make light-emitting diodes and laser diodes with a large range of emission wavelengths. More recently, InGaN alloys have also received attention for photovoltaic applications [1]. This interest is particularly motivated by *i)* the direct band gap (E_G) of these materials ranging from 0.64 eV for InN to 3.4 eV for GaN, and *ii)* the potential for integrated solutions with existing silicon technology. On the other hand, *p*-type character in In-rich InGaN is hardly obtained and the *p*-GaN/*i*-InGaN/*n*-GaN heterostructure is commonly used in photovoltaic cells. The difficulty in making devices with high In content active regions is partly related to the large lattice mismatch between InN and GaN, leading to the use of Multiple Quantum Well (MQW) [2]. This design raises questions about separation and transport of photo-generated electron-hole pairs.

Devices and Model

In this work, using quantum transport model, we compare a MQW with a thick-layer structure. The model is based on the Non Equilibrium Green Functions formalism with a two-bands (conduction and valence) effective mass Hamiltonian [3]. The electric potential, along the transport axe, is self-consistently calculated using Poisson's equation. Electron-phonon and electron-photon scatterings are both assumed within the self-consistent Born approximation. Photon incident flux is assumed to propagate along the electron transport direction with the spectra profile of the black-body at 6000K.

MQW device is defined by three quantum wells of 5 nm $In_{0.25}Ga_{0.75}N$ layers separated by 1 nm GaN barriers, while the thick-layer device has simply an active region of 15 nm of $In_{0.25}Ga_{0.75}N$. In both devices the active regions are embedded in doped GaN.

Results and Discussions

Band diagram and Local Density Of States (LDOS) are shown Figs. 1 and 2 for the MQW and the thick-layer solar cells respectively. We first see that band discontinuities induce peaked densities of states in both devices. In MQW, carriers are photo generated on localized states and then reach reservoirs only by tunneling and/or due to phonon scattering. In the thick-layer device, most of the states are directly contacted to reservoirs. However these delocalized states might absorb less photons since LDOS peaks in conduction and valence bands can be spatially remote (weak overlap).

Fig. 3 shows the illuminated *I-V* characteristics for both devices with and without phonon scattering. We first see that the current without phonons is slightly larger in the MQW than in the thick-layer. Fig. 3 also shows that characteristic for MQW is nonmonotonic and that incorporation of phonon scattering increases the current.

We now discuss these original results. Figs. 4 and 5 show current spectra calculated with phonon-scattering at *V*=0 V in both structures. As expected tunneling in MQW is of prime importance but it has also a non negligible impact in the thick-layer device. Tunneling being assisted by phonons [4], it explains why currents increase with scattering (Fig.3).

Fig. 6 shows the LDOS in MQW for the local current maximum obtained at *V*=1.5 V. At that bias, several localized states are aligned inducing a strong resonant tunneling. This effect could be at the origin of the nonmonotonic feature of the current characteristic in this structure.

References

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[3] N. Cavassilas *et al.*, J. Renewable Sustainable Energy **6**, 011203 (2014).
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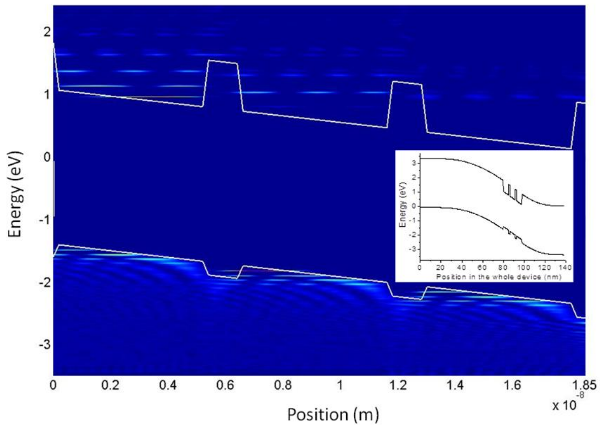

Fig. 1. LDOS in active region of the MQW solar cell.
Inset: band diagram in the whole device.
(N_A=5 10^{23} m^{-3}, N_D= 10^{24} m^{-3}, V=0 V).

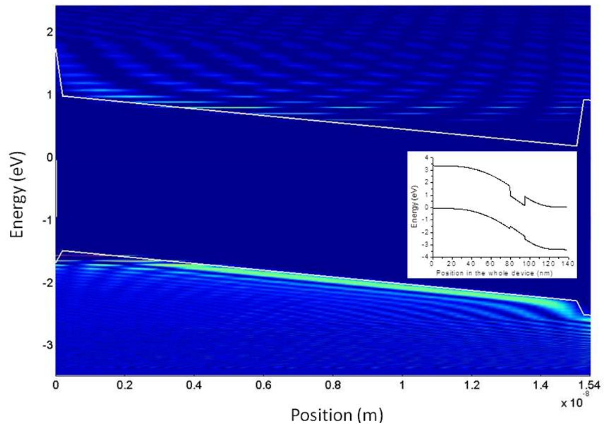

Fig. 2. LDOS in active region of the thick-layer solar cell.
Inset: band diagram in the whole device.
(N_A=5 10^{23} m^{-3}, N_D=10^{24} m^{-3}, V=0 V)

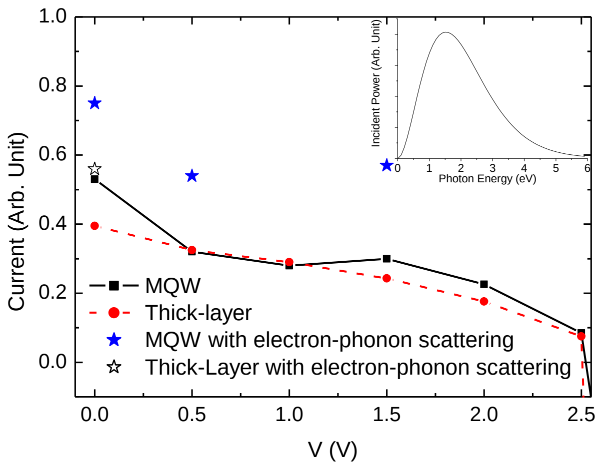

Fig. 3. Current characteristics for the two considered devices (MWQ and thick-layer) obtained without (squares and circles) and with (stars) electron-phonon scattering. Inset: considered solar incident power (black-body at 6000 K).

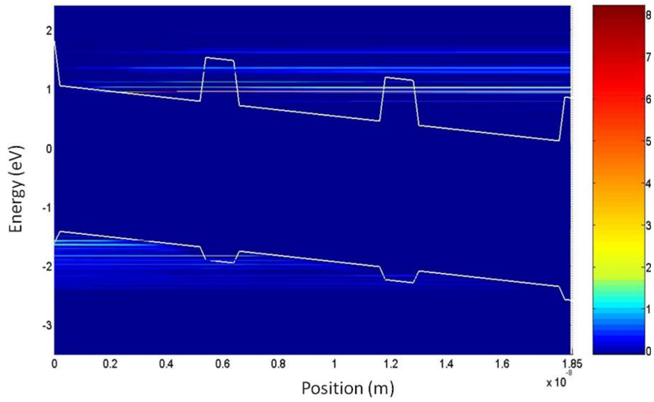

Fig. 4. Current spectra (in arbitrary unit) in active region of the MQW solar cell. (V=0 V)

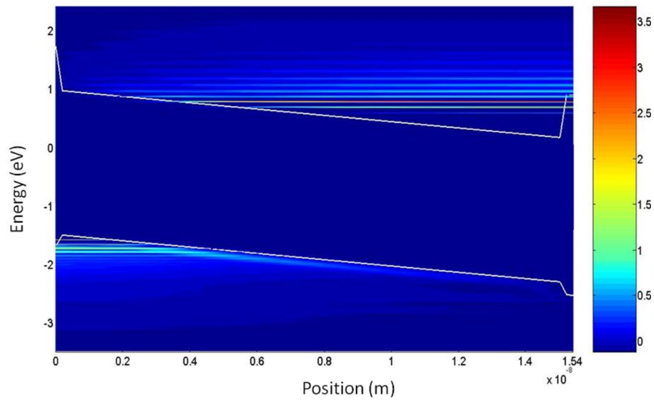

Fig. 5. Current spectra (in arbitrary unit) in active region of the thick-layer solar cell. (V=0 V)

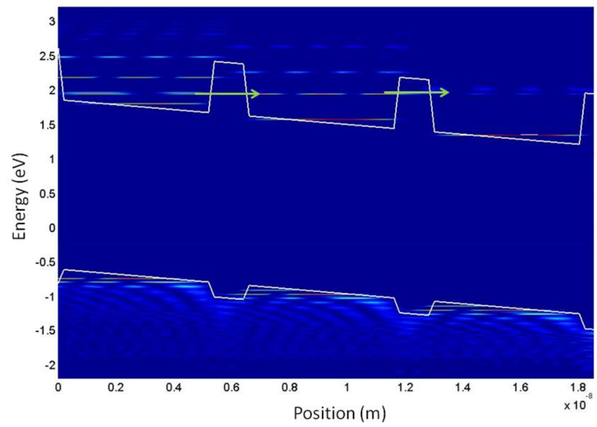

Fig. 6. LDOS in active region of the MQW solar cell. The green arrows represent the strong tunneling due to alignment of localized states in quantum wells. (V=1.5 V)