Thermionic escape in quantum well solar cell

Nicolas Cavassilas, Clémentine Gelly, Fabienne Michelini and Marc Bescond
Aix Marseille Université, CNRS, Université de Toulon, IM2NP UMR 7334, 13397, Marseille, France
e-mail: nicolas.cavassilas@im2np.fr

InGaN alloys are considered as promising candidates for high-efficiency photovoltaic devices, since their direct bandgap spans almost the whole solar spectrum from 0.64 eV (InN) to 3.46 eV (GaN). However, growing of high-quality InGaN layers with a large In content is difficult. Nevertheless, the synthesis of nanowires can be virtually substrate-free, which reduces the formation of dislocations [1].

We propose a theoretical investigation of InGaN/GaN core-shell nanowires for solar applications. The lattice mismatch between the InGaN and the GaN requires the use of multiple quantum wells [2] and limits both the In content and the thickness of the InGaN layers. Fig. 1 shows the calculated e_1-h_1 transition between the topmost hole energy level (h_1) and the deepest electron level (e_1) in an InGaN quantum well embedded in GaN barriers. This e_1-h_1 transition is represented as a function of the In content and the quantum well thickness t_{QW}. We also show a prohibited pink area representing the limit due to the lattice mismatch. The minimum e_1-h_1 transition obtained without any dislocation is 3 eV. These high-quality wells may be obtained if the GaN barriers are thick enough, *i.e.* ≥5 nm. In the following, we then propose to compare quantum wells exhibiting a e_1-h_1 transition equals to 3 eV with various In contents. These calculations are made with a photon energy of 3.2 eV, GaN barrier's thickness of 5 nm and 15 InGaN wells. No bias is applied.

The considered device and the corresponding calculated band-diagram are both represented in Fig. 2. This result is obtained with a 1D non equilibrium Green function formalism [3]. Electron-photon interaction is assumed in the central well of the device only. This permits to focus on the quantum efficiency of this particular well connected to the other parts of the device.

Fig. 3 shows the electronic Local Density of States (LDOS) obtained in the central quantum well for In contents of 14 and 19 % with corresponding t_{QW}=3.4 and 1.6 nm (devices A and B). In both devices electrons and hole are strongly localized in the quantum well since band offset between InGaN and GaN is high. A strong impact of the electron-phonon scattering on carrier extraction is thus expected. As shown in the insets of Fig. 3, this is confirmed by the secondary peaks located at $\pm\hbar\omega_{op}$ from the e_1 and/or e_2, where $\hbar\omega_{op}$=92 meV is the polar optical phonon energy. The major difference between both devices is the presence of the second state e_2 in the quantum well of device A. In device B, due to stronger confinement, the e_2 shift in the energy continuum.

Fig. 4 shows the photo-current spectra corresponding to the LDOS presented in Fig. 3. It results from phonon assisted thermionic escape as confirmed by the peaked shape of the spectra. Indeed, energy between peaks corresponds to $\hbar\omega_{op}$. The corresponding total currents are 83 and 3.8 (Arb. Unit) for devices A and B respectively. This unexpected ratio of about 20 has been established for several photon energies. Even if photon absorption depends on the thickness of the quantum well, the main reason of this high ratio is the thermionic escape. The rate of phonon absorption depends on the density of states of the final electronic energy. In device B, due to the strong confinement, density of states between e_1 and the continuum exhibits a minimum ~10^{-2} (Arb. Unit) as shown in the inset of Fig. 3. This minimum limits the phonon absorption of electrons and then their escape into the continuum. In device A, since the confinement is weaker, the minimum of density of states between e_1 and e_2 is higher (~10^{-1} Arb. Unit). Moreover, the state e_2, located between e_1 and the continuum, also contributes to the phonon absorption and finally to the thermionic escape.

[1] Y. Dong, B. Tian, T. J. Kempa, and C. M. Lieber, *Nano Lett.* 9, 2183 (2009).
[2] J. R. Lang, N. G. Young, R. M. Farrell, Y. R. Wu, and J. S. Speck, *Appl. Phys. Lett*. 101, 181105 (2012).
[3] N. Cavassilas, F. Michelini, and M. Bescond, *J. Renewable Sustainable Energy* 6, 011203 (2014).

ISBN 978-0-692-50554-0

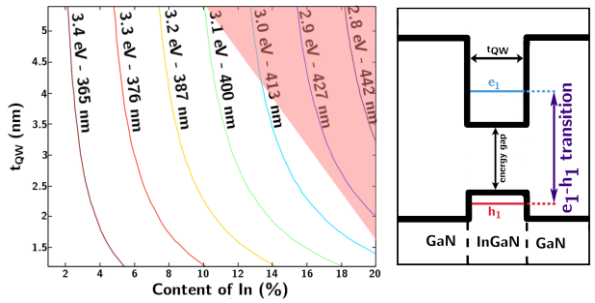

Fig. 1. Iso-energy curves for the e_1-h_1 transition *versus* the In content and the quantum well thickness t_{QW}. The pink area represents the conditions for which dislocations are expected.

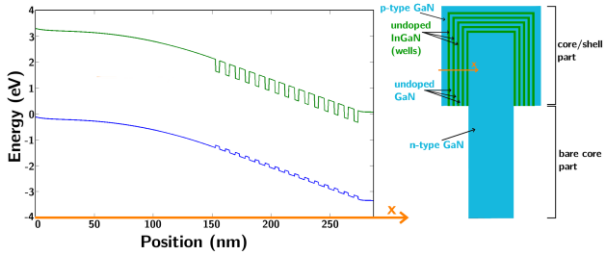

Fig. 2. Schematic representation of the considered core-shell nanowire and the corresponding 1D band-diagram obtained with V=0 V, N_A=7 10^{16} cm^{-3} and N_D=3.5 10^{18} cm^{-3}. The low electric field in the active region is due to the low p-doping.

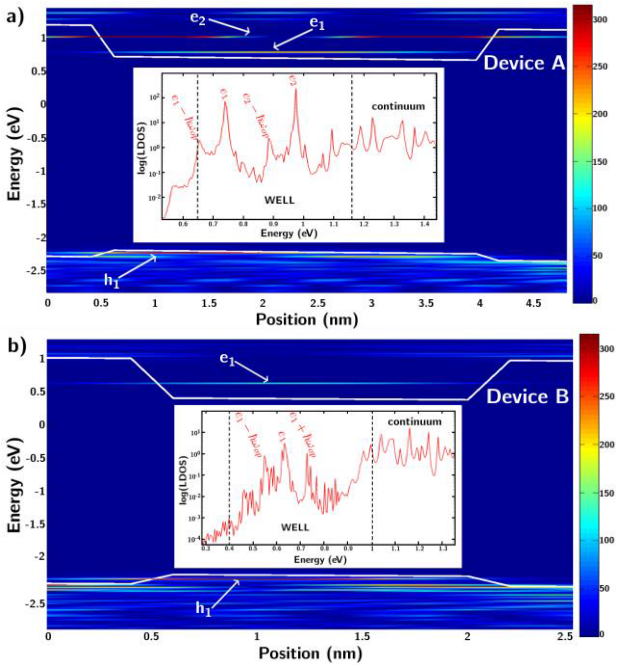

Fig. 3. The local density of states versus the energy and the position in central quantum well of devices with a) In content of 14 % and t_{QW}=3.4 nm (device A), and b) In content of 19 % and t_{QW}=1.6 nm (device B). The insets represent the corresponding integrated density of states in the conduction band versus the energy.

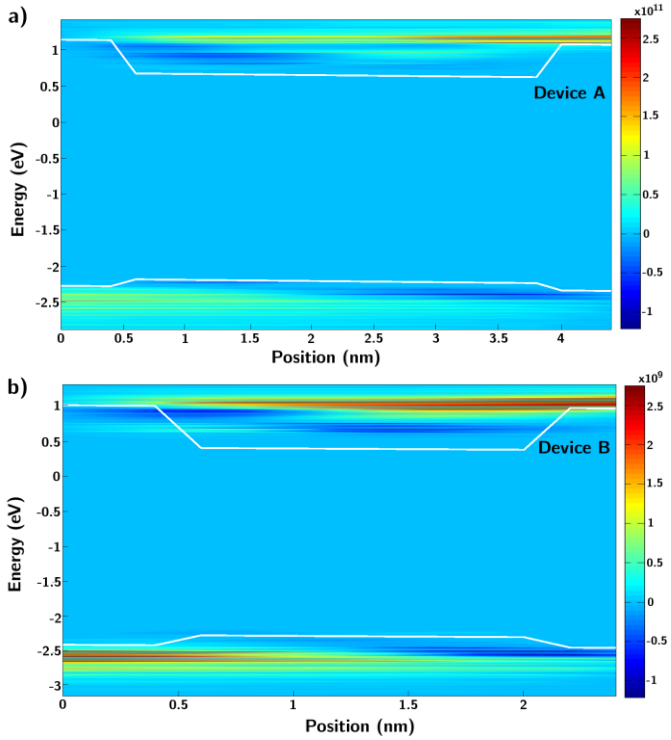

Fig. 4. Current spectra versus energy and position in the central quantum well of a) device A (In content of 14 %, t_{QW}=3.4 nm), and b) device B (In content of 19 %, t_{QW}=1.6 nm).