Quantum calculation of solar cell efficiency

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INTRODUCTION

Third-generation solar cells [1] based on quantum effects represent promising candidates to overcome the Schockley-Queisser limit [2]. Most of the solar cell simulations consider carrier transport from a semi-classical approach [3]. However, these models are no longer suitable to describe electronic transport in nano-structured devices. So far, few quantum simulations have been reported [4]. These models, computationally challenging, have been applied to specific studies with generally a monochromatic incident light. However, assuming the entire sun spectrum is essential to model solar cells and calculate the power conversion efficiency (PCE). We present a quantum transport model considering the black-body spectra for the incident light. Inspired by the excellent results achieved by *Alta Device* [5], we focus on thin GaAs *p-i-n* junctions. We analyze the different negative contributions to photovoltaic (PV) current *versus* the applied voltage.

DEVICE and MODEL

The considered GaAs *p-i-n* junction is detailed Fig. 1. The invariance of the potential in the transverse plan permits to separate the 2D dispersion from the 1D transport. The 1D transport modelling is based on the non-equilibrium Green's function formalism with two one-band effective mass Hamiltonians (conduction and valence) coupled by the electron-photon interaction. The 1D electric potential is self-consistently calculated using Poisson's equation. Electron-phonon scattering is included through polar optical phonon interactions. Photon incident flux is assumed to propagate along the electron transport direction with a power P_{sun}=1000Wm^{-2} (AM1.5 Global standard) and the spectra profile of the black-body at 6000K. In electron-photon interaction we assume a decrease of the light intensity according to an absorption coefficient of 2.7 10^{4}cm^{-1}.

RESULTS and DISCUSSION

Figure 2 shows the current characteristics *J-V* and the corresponding power (P=$J.V$) obtained without phonon scattering. These results agree rather well with experimental results [6]. The PV current is maximum for V=0. The corresponding spectra is shown Fig. 3 *versus* position along the transport direction. In addition to the expected positive current we show a negative contribution at the device edges (labeled as LEC for Large Energy Contribution). Carriers generated at energy larger than the junction barrier are less sensitive to electric field and may reach the wrong contact. The power is maximum for V=0.75V with a PCE (P/P_{sun}) of 20.9%. For that bias, the LEC increases with respect to V=0 due to the reductions of both the electric field and the junction barrier (Fig. 4). In spirit of the *Alta Device* cell [5], $Al_{0.38}Ga_{0.62}As$ is used in the *p*-type extremity. This allows to reduce the LEC for electrons and PCE reaches 22.3% (Fig. 5). For larger bias (*e.g.* V=0.85 V) the power is strongly reduced. As shown in Fig. 6, the current spectrum depicts the emergence of a new negative contribution (labeled as MRC for Majority Recombination Contribution) which vanishes when switching-off the photon emission. Due to the low electric field, majority carriers reach the central region and recombine radiatively. It follows a negative current of majority carriers. Finally, phonon scattering incorporation reduces PCE maximum down to 16.5% (against 20.9%).

In conclusion, this study highlights two behaviors limiting the efficiency of thin solar cells. While the MRC is expected to be reduced in a thicker junction, we clearly show that the LEC can be reduced by the use of an heterojunction.

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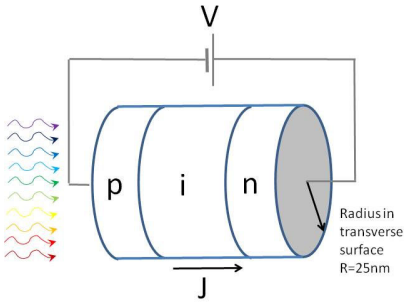

Fig. 1. Schematic representation of the considered *p-i-n* junction (N_D=N_A=10^{25}m^{-3}, L_n=L_p=10nm, L_i=160nm). The transport axis is discretized (Δx=0.2nm), as well as the transverse wave vector **k** (Δk=π/R). For GaAs we assume an energy band-gap Eg=1.43eV, and effective masses of the valence and conduction bands equal to m_v=0.51m_0 and m_c=0.07m_0 respectively (m_0 being the free electron mass).

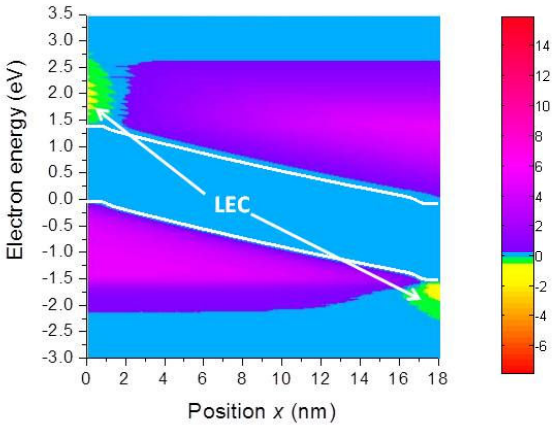

Fig. 3. Current spectra (in arbitrary units) *versus* position along transport axis x for V=0V. Valence and conduction band-edges are also shown (white lines).

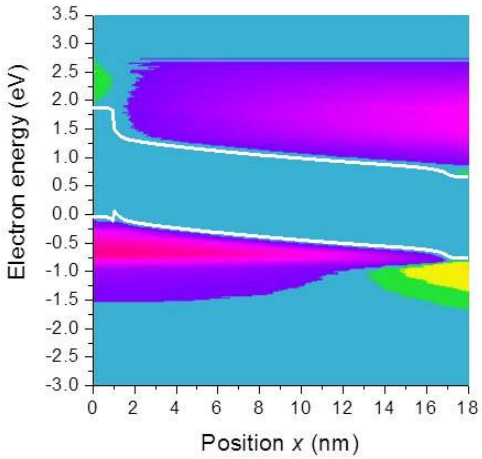

Fig. 5. Like Fig. 3 with V=0.75 V and $Al_{0.38}Ga_{0.62}As$ added at the p-type material extremity. For the AlGaAs/GaAs heterojunction we took bands offset given by ΔE_c=0.3eV and ΔE_v=0.19eV.

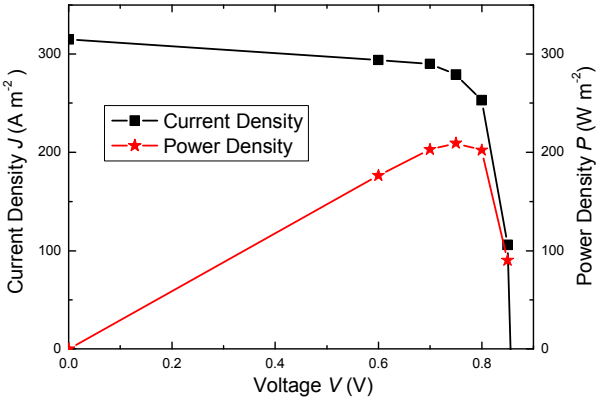

Fig. 2. Current-density J *versus* applied voltage V obtained without phonon scattering and the corresponding generated power density P.

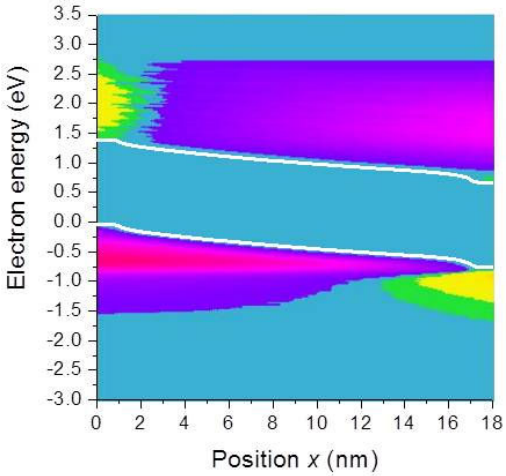

Fig. 4. Like Fig. 3 with V=0.75V.

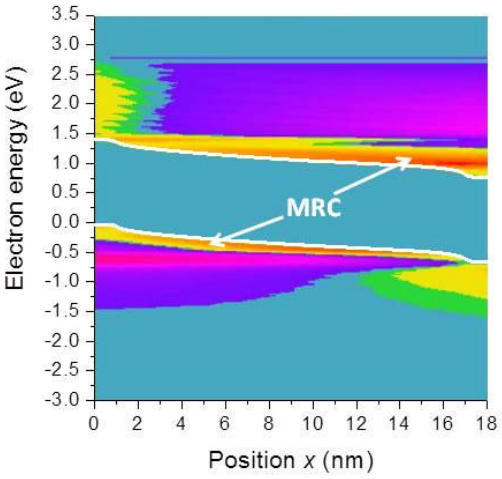

Fig. 6. Like Fig. 3 with V=0.85V.