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Modeling of type-II quantum dot intermediate band solar cells accounting for thermal and optical intersubband transitions

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***Abstract*—Novel solar cell concepts relying on the use of nanostructures requires *ad hoc* device modeling tools able to cope with carrier transport and charge transfer mechanisms involving the host bulk material and the quantum confined states. In this work we apply such approach to study the implication of intersubband competitive processes in type-II GaSb/GaAs quantum dots on their application to intermediate band solar cells.**

Quantum dots have been investigated since several years for demonstrating intermediate band solar cells (IBSC) [1]. Intraband transitions enabled by the 3D confinement allow the so-called two photon absorption (TPA) process producing an extra photocurrent while maintaining a high photovoltage, resulting in a theoretical efficiency well above that one of single junction cells. Type-I InAs/GaAs QDs have been very extensively studied and the IBSC operating principles proven. However, temperature-assisted intraband escape processes compete with the second photon absorption to such an extent that observation of TPA generally requires cryogenic temperatures, and the reported QD cells usually work in a thermally-limited operating regime. On the other hand, models of IBSCs [2] usually neglect thermally activated transistions, and thus have limited application to the analysis and design of practical devices. To fill this gap, we have recently proposed a drift-diffusion based model of QD solar cells which includes a proper treatment of quantum carrier capture and escape [3] and proven its ability to explain inherent limitations and experimental results of InAs/GaAs QD solar cells [4], [5].

In this work, we apply the model to study IBSCs based on GaSb/GaAs QDs (see Fig.1), whose intersubband dynamics are more promising than those of the InAs/GaAs QDs in view of attaining the IB operating regime. In fact, GaSb/GaAs QDs are characterized by high energy confinement in the valence band (VB) (between 0.4 and 0.49 eV [6]–[9] and by staggered band alignment (type-II, see Fig.1(b)). The reduced overlap between electron and hole wavefunctions causes a carrier radiative lifetime on the order of 10 ns [10], [11], about ten times larger than that one of InAs/GaAs QDs.

The impact of the GaSb/GaAs QDs on the electrical performance of IBSCs is studied based on the simple $p-i-n$ structure shown in Fig.1(a), which includes 5 QD layers within a 100 nm thick intrinsic region. The assumed GaSb/GaAs QD parameters are summarized in Table I.

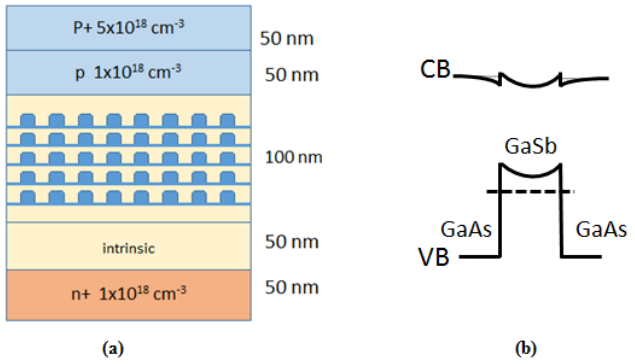

Fig. 1. (a) The solar cell structure used in the simulation. (b) GaSb/GaAs quantum-dot with staggered band alignment.

TABLE I
TYPE-II GASB/GAAS QD PARAMETERS

QD in-plane density [cm^{-2}]	1×10^{11}
$\Delta E_{\text{VB-GS}}$ [eV]	0.25-0.40
$\tau^{h}_{\text{CAP,VB-GS}}$ [ps]	5 [12]
τ_r^{GS} [ns]	10
GS degeneracy	6
$\alpha_{\text{IB}\rightarrow\text{CB}}$ [cm^{-1}]	10^3
$\alpha_{\text{IB}\rightarrow\text{VB}}$ [cm^{-1}]	10^4

The device is analyzed by a 1D drift-diffusion model completed by a rate equation that links the 3D bulk carrier densities to the QD confined carrier densities in each dot layer [3]. according to the schematic model shown in Fig.2, which describes the interband radiative transistions ($G_{\text{ph}}^{\text{BB}}$, and $R_{\text{QD}}^{\text{rad}}$) and the intersubband net thermal ($R_{ESC}^{Thermal}$) and radiative (G_{ph}^{2nd}) escape processes. QD layers are assumed uncoupled to the large interdot layer thickness.

Fig.3 shows the calculated net thermal and TPA escape rates for different QD confinement energy, highlighting the suppression of thermal emission as the confinement energy increases and the onset of dominat optical emission at high concentration in agreement with the results in [13]. The thermally-limited and IB operating regime for the cells with shallow and deep confinement QDs, respectively, is shown

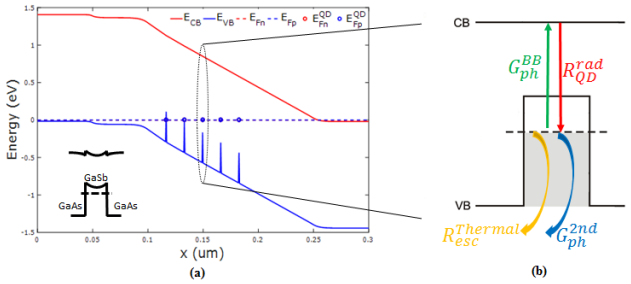

Fig. 2. (a) Thermal equilibrium band diagram of the cell under study. (b) QD model with relevant interband and intersubband transistions.

in Fig.4. The thermally limited regime is chracterized by a logarithmic dependence of V_{oc} on the sun concentration (XSUN) - according to the diode equation in radiative limit -, whereas the IB operating regime is characterized by a stronger dependence of V_{oc} on concentration, confirming the theoretical predictions in [2] which were derived neglecting thermally activated escape. In fact, in the IB regime a larger carrier injection is needed to compensate for the increase of TPA-driven escape as the concentration increases.

Going further, and exploring the use of QD doping and the possibility to enhance the TPA by light-trapping approaches [14], simulations shows that cells with deeply confined QDs the onset of truly IB regime can be pursued at markedly lower concentrations, on the order of tens of sun.

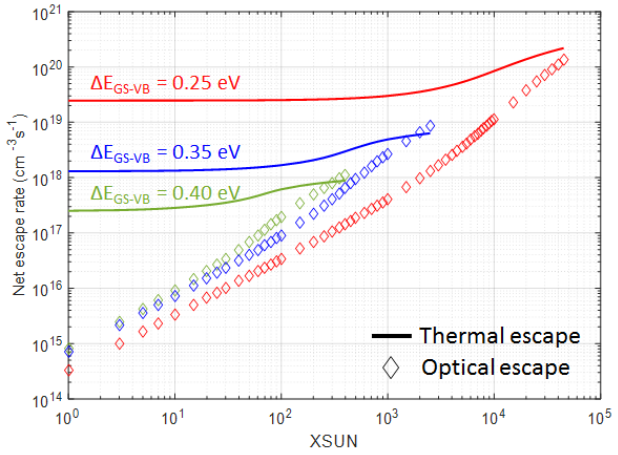

Fig. 3. Thermal and optical emission rate of charges from the GS to the VB continuum, considering confinement levels of 0.25, 0.3 and 0.4 eV within the VB.

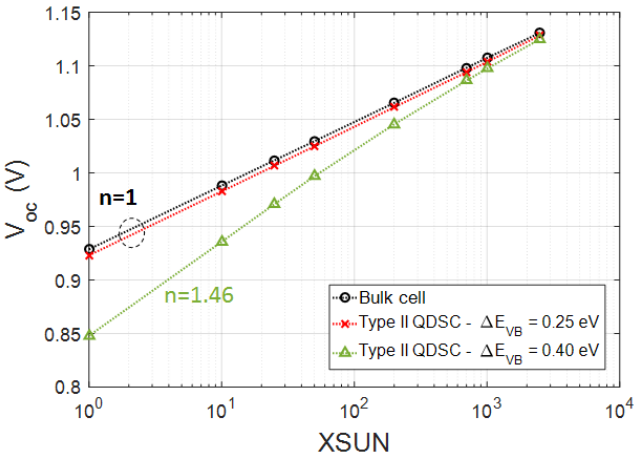

Fig. 4. Evolution of open circuit voltage with respect to sun concentration for QDSC with Type-II band alignment with shallow (0.25 eV) and deep (0.4 eV) confinement within the VB. The open circuit voltage behavior of the bulk cell is also shown.

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