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Original

Study of light-trapping enhanced quantum dot solar cells based on electrical and optical numerical simulations / Cappelluti, Federica; Musu, Antonio; Khalili, Arastoo. - ELETTRONICO. - (2016), pp. 1-2. (Intervento presentato al convegno 2016 Compound Semiconductor Week, CSW 2016 tenutosi a Toyama, Japan nel 2016) [10.1109/ICIPRM.2016.7528629].

Availability:

This version is available at: 11583/2655932 since: 2016-11-15T13:40:14Z

Publisher:

Institute of Electrical and Electronics Engineers Inc.

Published

DOI:10.1109/ICIPRM.2016.7528629

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Study of Light-Trapping Enhanced Quantum Dot Solar Cells based on Electrical and Optical Numerical Simulations

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Abstract—We study InAs/GaAs quantum dot solar cells exploiting light trapping approaches to enhance the interband light harvesting efficiency of quantum dots. A realistic thin-film structure including a nanostructured anti-reflection coating and a planar reflector is investigated both from the optical and electrical standpoint, based on finite difference time domain electromagnetic simulations and on quantum-dot-aware transport simulations. The photovoltaic efficiency of quantum dot solar cells and reference bulk cells is analyzed for various configurations, from the single-pass -wafer-based- one to the thin-film one approaching the ideal Lambertian limit. We show that light-trapping enhancement, combined with QD selective doping, may allow the quantum dot cell to achieve photovoltaic efficiency higher than its bulk counterpart.

Keywords— *solar cell, quantum dot, thin film, doping, light trapping, nanophotonic*

I. INTRODUCTION

It is well known that InAs/GaAs Quantum Dot (QD) Solar Cells suffer from a limited light harvesting of the QD material, which - together with a usually remarkable penalty of the open circuit voltage –prevents them from overcoming the photovoltaic efficiency of single-junction cells. A possible path to circumvent this issue is to exploit photon management via light-trapping effects in order to enhance the QD absorption length [1]. In particular, periodic nanophotonic gratings can be implemented within a thin-film configuration (i.e. removing the substrate, e.g. through wafer epitaxial lift-off [2]) to achieve effective light-trapping. In this work, we investigate the potentiality of such an approach by studying, through rigorous electromagnetic and physics-based simulations [3], a realistic device configuration of InAs/GaAs QD cells aimed at implementing effective light-trapping.

II. RESULTS

As sketched in Fig. 1, the thin-film device combines a nanostructured periodic grating on the top with a planar reflector at the rear side. The periodic grating has the twofold role of acting as broadband antireflection coating (ARC), with very low reflectivity in the 400-1200 nm range, and of exciting higher diffraction modes in the cell for achieving light-trapping in a wavelength range of about 800-1100 nm (covering the GaAs band edge and QD interband transitions). The presented results refer to the ARC-optimized geometry realized in [4], with nanocone size features of 80/300/440 nm (top radius /base radius /height). We estimated the cell reflectivity (Fig. 2) and absorption enhancement (Fig. 3 and Table 1) in the GaAs/QD active region, through Finite Difference Time Domain (FDTD) simulations. Fig. 3 compares the absorbed photon density for various device configurations: i) a conventional -wafer-based- single-pass cell with planar ARC; ii) a – wafer based- cell with nanostructured ARC (the nanocone grating); iii) a thin-film cell with nanostructured ARC and ideal reflector (modeled as perfect electrical conductor). The conventional exponential decreasing photogeneration in i) is replaced by significant coherence patterns in ii) and iii) configurations. As highlighted in Table 1, both ii) and iii) configurations provide gain in the total absorbed photon density. At 900 nm (GaAs absorption length ~ 0.1 cm), configuration iii) allows for doubled photogeneration. The impact of doubled effective absorption length on the external quantum efficiency is analyzed in Fig. 5. As upper limit, we also report the behavior at the Lambertian limit (full LT, corresponding in the 1D simulation presented here to a maximum path length enhancement of about $2n^2=25$ for GaAs). Finally, in Fig. 6 we investigate to what extent the achievable conversion efficiency may be improved by doping optimization, through uniform doping density in the intrinsic region of the reference cell and direct doping in the QD cell. The QD cell with optimized doping shows efficiency comparable to the optimized bulk one in the double pass configuration and an absolute improvement of about 0.8 % in the Lambertian limit.

III. ACKNOWLEDGEMENTS

This project has received funding from the European Union's Horizon 2020 research under Grant Agreement 687253 - TFQD.

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Fig. 1. Sketch of the investigated solar cell exploiting nanostructured ARC and reflector and detailed cross-section of the QD/GaAs region. Note that p^+ GaAs-contact layers and metal layers are not shown.

Fig. 2. Simulated reflectivity of a planar AlInP/GaAs structure and nanostructured AlInP/GaAs structure.

Fig. 3. (a) 3D distribution of the absorbed photon density at $\lambda=900$ nm for the structure exploiting nanocone ARC and planar reflector. (b), (c) Cutline across the z -axis of the absorbed photon density at $\lambda=830$ nm and $\lambda=900$ nm, respectively, for various structures: i) planar ARC w/o reflector, ii) nanocone ARC w/o reflector, iii) nanocone ARC with planar reflector.

Table 1. Estimated Gain in the total absorbed photon density of the solar cells exploiting the nanostructured ARC with and w/o reflector with respect to the conventional cell (with planar ARC and no reflector), for wavelengths below (830 nm) and above (900 nm) the GaAs band edge.

Structure	Normalized Integrated Absorbed Photon Density	
	830 nm	900 nm
Planar ARC w/o reflector	1	1
Nanocone ARC w/o reflector	1.2	1.3
Nanocone ARC with reflector	1.4	2.7

Fig. 4. (a) Calculated energy band diagram of the device shown in Fig.1 at thermal equilibrium (a), and short circuit condition under 1 sun AM1.5G illumination (b). For the sake of electrical simulations, a thin p^+ GaAs-contact layer is included. The intrinsic region embeds 20 QD layers with density of $6 \times 10^{10} \text{ cm}^{-2}$.

Fig. 5. Calculated External Quantum Efficiency (EQE) for the REF cell for single-pass and full light-trapping configurations, and for the QD cell for single-pass, double-pass and full light-trapping configurations.

Fig. 6. Power conversion efficiency vs. doping density for the REF and QD cells in the single-pass and full light-trapping configurations. The doping density in the bulk cell is equal to $\alpha \times 1.2 \times 10^{16} \text{ cm}^{-3}$.