Electro-Optical Modeling of InP Nanowire Solar Cells: Core-shell vs. Axial Structure

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***Abstract*—We present an investigation of the photovoltaic effect in InP nanowire arrays for both axial and core-shell structures. A microscopic electro-optical model is used to analyze the current-voltage relationships and cell efficiencies. It is found that core-shell structures provide a larger photocurrent and efficiency yet lower open circuit voltage than an axial structure. The analysis of the p-n junction operation explains this difference and gives design guidelines for nano-photovoltaic devices.**

I. Introduction

Semiconductor nanowire solar cells have been gaining broad attention recently. Compared to traditional thin-film devices, nanowires have much better tolerance for lattice mismatch, and therefore provide the possibility to use inexpensive substrates for III-V devices and great flexibility in the bandgap choice for multi-junction arrangements [1]. In this paper, the carrier generation efficiency of nanowires in an axial and core-shell configuration is studied, and from an analysis of the internal device physics, the carrier collection mechanisms and their impact on the current-voltage relationships in both arrangements is explained.

In our simulations, we choose 2 μm long single junction InP nanowires with $5 \times 10^{18} cm^{-3}$ n-doping and $1 \times 10^{18} cm^{-3}$ p-doping. The distance between neighboring nanowires' central axes in the infinite array is set to 400 nm. The axial structure consists of a 160 nm diameter nanowire with a 100 nm thick n-doped layer as the emitter. The core-shell structure is a 160 nm diameter nanowire with a p-doped core of 100 nm diameter, with the lateral and axial thickness of the n-doped outer shell being 30 nm and 100 nm, respectively [2] (see Figure 1).

The optical generation is calculated by solving Maxwell's equations in three dimensions, with a plane-wave illumination representing an unconcentrated AM1.5D solar spectrum [3]. The generation is shown in Figure 1. Due to the highly dispersive nature and strong absorption of the nanowire array, the spectrally integrated optical generation is concentrated in the top area of the wires, with an exponential decay to the bottom. Furthermore, the generation increases radially towards the wire surface. Details can be found in [3].

The electronic simulation consists of the solution of a 3-dimensional drift-diffusion/Poisson system using the method developed in [4]. Both radiative and non-radiative recombination is included, and the continuity equations contain spatially resolved generation terms according to Fig. 1. Due to the large diameter of 160 nm of the wires, quantization effects are neglected at this stage of analysis.

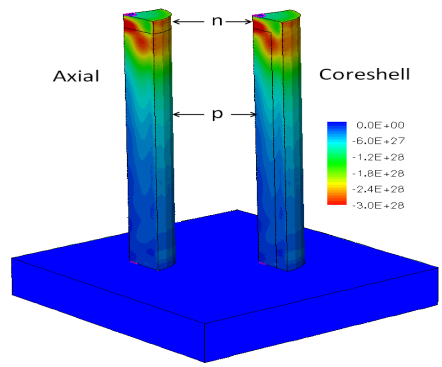

Fig. 1: Device geometry of a quarter of axial (left) and core-shell (right) nanowire, n and p regions are indicated, the optical generation distribution is also given.

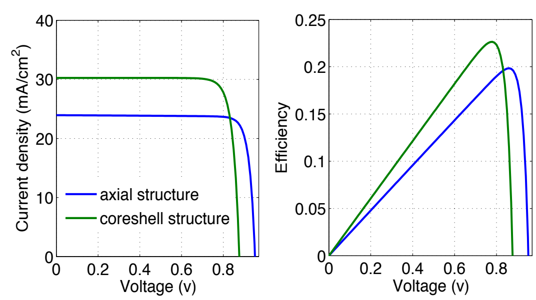

Fig. 2: Current vs. voltage (left) and efficiency vs. voltage (right) of axial and core-shell nanowires under AM1.5d illumination

II. Device Analysis

A. Current-voltage relationships and efficiencies

Figure 2 shows the current and efficiency vs. voltage characteristics of the axial and core-shell array under AM1.5d unconcentrated illumination. The maximum efficiency (η_{max}) of the core-shell structure is 22.64%, and η_{max} of the axial structure is 19.84%. The short circuit current density (I_{sc}) of the axial nanowire is $23.94 mA/cm^2$, while for core-

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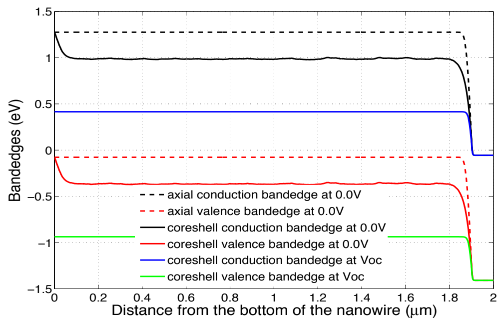

Fig. 3: Conduction and valence bands of axial and core-shell nanowire along the central axis under AM1.5d illumination.

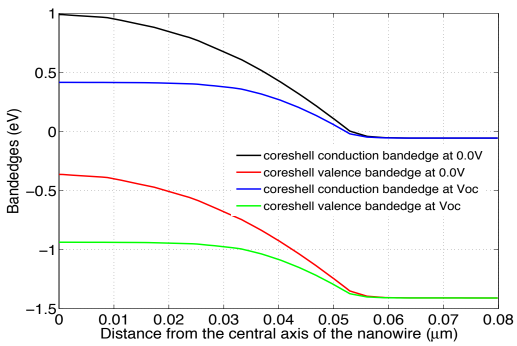

Fig. 4: Radial cut of the conduction and valence bands for core-shell nanowire under AM1.5d illumination. The distance from the nanowire's bottom is 400nm .

shell structure, $I_{sc} = 30.26mA/cm^2$, which shows that a larger photocurrent is produced by the core-shell structure. Eventually, this leads to a larger η_{max}, however, the open circuit voltage (V_{oc}) of the axial nanowire is larger (0.95V vs. 0.88V in the core-shell case).

B. Discussion

The major difference between the axial and core-shell nanowire is the location of the p-n junctions, i.e. the depletion zones.

The axial structure is similar to a traditional thin film single junction device, with a depletion zone extending along the central axis. The core-shell structure, in which a lateral junction is introduced, has a depletion zone expanding in three dimensions, see Figure 1.

Figure 3 shows the valence and conduction bands of the axial nanowire along the central axis at short circuit operation and the bands of the core-shell structure at short circuit and open circuit condition. At the short circuit current, the depletion zone extends approximately 100 nm into the p-region, and leads to a built-in potential of 1.3 V. This potential fully drops at $z = 1.9\mu m$ in the axial case, as only one junction is present. For the core-shell case, the total voltage drop is divided in two parts: a voltage drop A happens at the axial depletion zone of the structure. The p-core radius is smaller than the p-depletion width, hence the core is only partially depleted (see Fig. 4). Due to this partial depletion, potential drop at A ends at the level of the radial potential arising from the partial depletion. The remaining voltage drop B is located in the depletion zone between the p-contact and the radial junction on the bottom of the wire. This effect can potentially decrease the cell performance, as the axial junction (which is the main junction for photogeneration) has a reduced depletion width. From the optical generation field calculation, most generation happens at the top and outer shell of the nanowire, so the extra radial depletion region in the core-shell structure enhances the effective separation of generation carriers. The photocurrent increases as a result (see Figure 2).

At open circuit voltage condition (V=0.88 V), the potential drop at location B has been compensated by the applied forward voltage (see Fig. 3), therefore, the top junction of the core-shell structure is biased identically to the axial structure. The reduction of the open-curcuit voltage in the core-shell case can be explained as follows: the open circuit voltage is the operation voltage at which the forward current of the solar cell compensates the (reverse) photo-current generated by illumination. In the axial case, the forward current is generated in a horizontal cross-section of the wire which is fully illuminated. In the core-shell case, the forward current is generated both in the axial junction and in the radial junction equally (the same voltage is applied at both). The latter has a large junction area, and does not contribute photo-current to equal parts due to the exponentially decreasing generation at the bottom of the wire. Therefore, the open circuit voltage is achieved at smaller bias values compared to the axial structure.

III. Conclusion

Both axial and core-shell single junction InP nanowires provide maximum efficiencies of around 20%, which is close to their thin-film counterparts. In the core-shell structure, the core region can be used for charge separation and I_{sc} is enhanced by 20% due to the effect of the lateral junction. The lateral junction however also has a strong impact on V_{oc} under external bias. These mechanisms give guidelines for the optimum design of a core-shell nanowire solar cell with respect to doping levels and lateral dimensions.

Acknowledgment

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