Numerical Analysis and Device Optimization of Radial p-n Junction GaAs/$Al_xGa_{1-x}As$ Core-Shell Nanowire Solar Cells

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Abstract - Based on the transfer-matrix method and the complex wave impedance approach, this unified electrical and optical numerical simulation thoroughly analyzes the impacts of the design parameters on the transport mechanisms and device characteristics of radial p-n junction GaAs/$Al_xGa_{1-x}As$ core-shell nanowire solar cells. By optimizing the doping density of the core and shell, core radius, shell thickness, nanowire length as well as the Al mole fraction of the n-type $Al_xGa_{1-x}As$ shell, the optimized device exhibits an open-circuit voltage of ~0.94V, a short-circuit current of ~55.5 pA (effective short-circuit current density is ~40.9 mA/cm^2), and a fill-factor of ~0.76. Hence, this clearly shows that radial p-n junction GaAs/$Al_xGa_{1-x}As$ core-shell nanowire solar cell on Si substrate is capable of achieving an unprecedented solar cell efficiency of ~30% for single-junction GaAs solar cells in a cost-effective way.

I. INTRODUCTION

Recently, radial p-n junction core-shell nanowire solar cells [1]-[6] have attracted a lot of attention because this device architecture enables effective light absorption and efficient carrier collection to be achieved simultaneously. This feature is unique to the radial p-n junction core-shell nanowire structure because absorption of sunlight takes place axially along the core of the nanowire whereas the collection of photo-generated carriers happens radially out of the core of the nanowire. Apart from that, nanowire array inherently exhibits enhanced light absorption due to their intrinsic light trapping effects and reduced light reflection without using anti-reflection coatings. Therefore, it is expected that the radial p-n junction core-shell nanowire structure could achieve higher solar cell efficiencies that cannot be obtained using the planar device geometry. The nanowire device concept also offers an additional cost advantage because III-V compound semiconductor nanowires can be grown directly on cheaper substrates. Hence, radial p-n junction III-V compound semiconductor core-shell nanowires would make it possible to develop low-cost and high-efficiency solar cells. However, despite the above advantages of the radial p-n junction core-shell nanowire structure, the reported solar energy conversion efficiencies for radial p-n junction core-shell nanowire solar cells are less than 10% [3]-[6] when illuminated with the one-sun AM1.5G solar spectrum regardless of the material system used. Clearly, something must be amiss and it is the aim of this work to gain insights into improving the solar energy conversion efficiency of radial p-n junction GaAs/$Al_xGa_{1-x}As$ core-shell nanowire solar cells.

The approach taken in this numerical study is to vary the doping density of the core and shell, core radius, shell thickness, nanowire length, and Al mole fraction of the $Al_xGa_{1-x}As$ shell to study the influences of these design parameters on the device characteristics of these unique devices. This finite-element analysis was based on the transfer-matrix method and complex impedance approach, and the simulations were performed using a commercial technology-computer-aided-design package called Sentaurus.

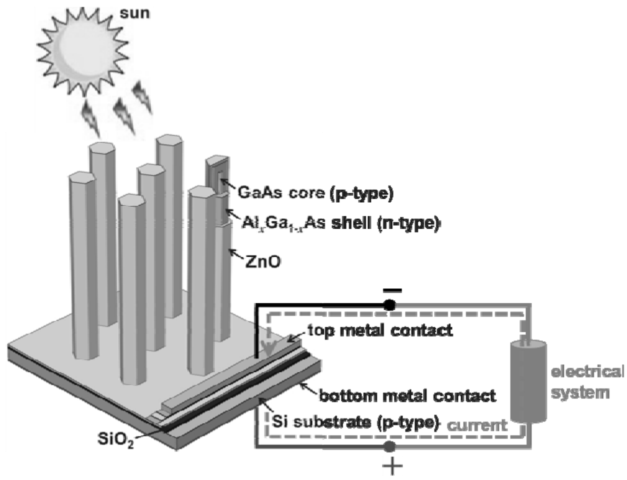

Fig. 1. Schematic diagram showing the device structure of a radial *p-n* junction GaAs/$Al_xGa_{1-x}As$ core-shell nanowire solar cell.

II. RESULTS AND DISCUSSIONS

An example of the radial p-n junction GaAs/$Al_xGa_{1-x}As$ core-shell nanowire solar cells analyzed in this study is shown in Fig. 1. In order to keep the computation loads manageable, only a single radial p-n junction GaAs/$Al_xGa_{1-x}As$ core-shell nanowire was considered and light-trapping effects were excluded in the simulations. The focus of the initial simulations was on studying the effects of the doping densities of the core and shell on the device characteristics. For this purpose, a value of 100 nm was considered for the core diameter and shell thickness, and the solar cell efficiency for a radial p-n junction GaAs/$Al_{0.2}Ga_{0.8}As$ core-shell nanowire solar cell as a function of the core and shell doping densities are shown in Fig. 2. Clearly, the result showed that the combination of a high core doping density and low shell doping density would lead to high solar cell efficiencies. That is because higher core doping with lower shell doping leads to larger quasi-Fermi-level splitting and stronger electric field. Consequently, open-circuit voltage and short-circuit current improved considerably and resulted in higher solar cell efficiencies. In this result, an optimum solar

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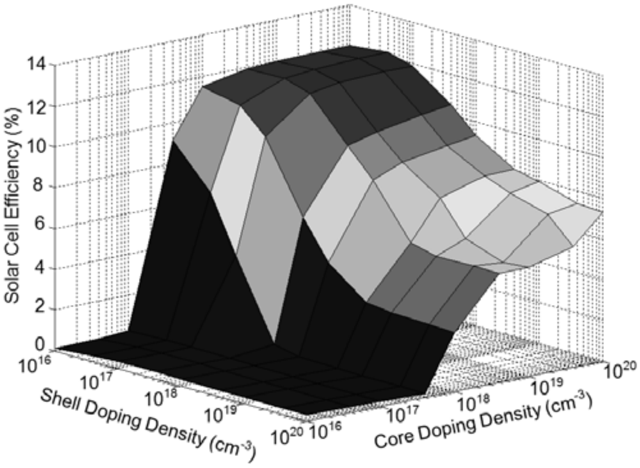

Fig. 2. Solar cell efficiency of the radial *p-n* junction GaAs/$Al_{0.2}Ga_{0.8}As$ core-shell nanowire versus doping densities of the *p*-type GaAs core and *n*-type $Al_{0.2}Ga_{0.8}As$ shell under one-sun AM1.5G solar spectrum illumination. The core diameter, shell thickness, and nanowire length were 100 nm, 100 nm, and 3 μm, respectively. The Al mole fraction of the $Al_xGa_{1-x}As$ shell was 0.2.

cell efficiency of ~12.2% was achieved with core doping density of at least 4×10^{19} cm^{-3} and a shell doping density of 4×10^{16} cm^{-3}.

Next, the core and shell doping densities were kept constant at 4×10^{19} cm^{-3} and 4×10^{16} cm^{-3}, respectively, to examine the effects of the core radius and nanowire length on the solar cell efficiency of the radial p-n junction GaAs/$Al_{0.2}Ga_{0.8}As$ core-shell nanowire solar cells. As can be observed from the results shown in Fig. 3(a), the solar cell efficiency increased with increasing nanowire length due to absorption of deep penetrating spectral components and the optimum solar cell efficiency at each nanowire length was achieved at a core radius of around 200 nm as a consequence of optimal spectral overlap between the optical mode of the nanowire and the AM1.5G solar spectrum. Hence, the core radius was kept constant at 200 nm in the subsequent simulations to determine the optimum nanowire length for achieving the optimal solar cell efficiency for the radial p-n junction GaAs/$Al_{0.2}Ga_{0.8}As$ core-shell nanowire solar cells. As a result, it was found that the solar cell efficiency increased to ~30% for a 6 μm-long nanowire, but dropped to ~20% for a 7 μm-long nanowire because of hole pile-up which caused excessive non-radiative recombination in the core. Finally, evaluation of the effects of Al mole fraction in the $Al_xGa_{1-x}As$ shell showed that solar cell efficiency increased with increasing Al mole fraction due to larger quasi-Fermi-level splitting and strong electric field. It was found that the solar cell efficiency peaked at an Al mole fraction of 0.2 and decreased substantially for Al mole fractions above 0.2 due to the increasing large conduction-band energy barrier at the heterojunction which limited current flow.

IV. Conclusion

It has been shown in this study that single radial p-n junction GaAs/$Al_{0.2}Ga_{0.8}As$ core-shell nanowire solar cells are capable of surpassing the ~28 % solar cell efficiency achieved with the current best single-junction planar thin-film GaAs solar cell. It is envisaged that solar cell efficiencies higher than 30% could be possible with these unique solar cells by optimizing the light-trapping effects of these unique solar cells and fabricating

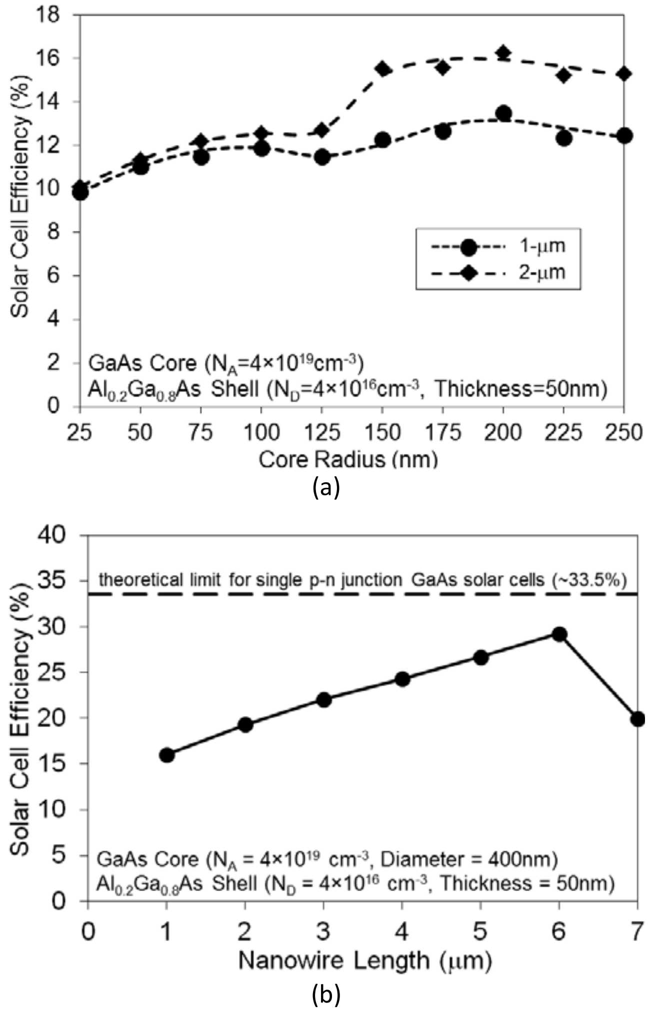

Fig. 3. (a) Solar cell efficiency of the single radial *p-n* junction GaAs/$Al_{0.2}Ga_{0.8}As$ core-shell nanowire as a function of the (a) *p*-type GaAs core radius and (b) nanowire length when its top facet was under one-sun AM1.5G solar spectrum illumination.

these unique solar cells on highly conductive materials.

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