GaAs truncated cone nanowire array-based solar cells with carrier selective contacts

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***Abstract*—Recent advancements in solar cell technology have unveiled the potential of nanowire (NW) structures, particularly those incorporating III-V materials, for enhanced light absorption and reduced material consumption compared to traditional planar designs. Our research introduces a novel core-shell heterojunction design featuring a p-type GaAs truncated cone NW core and Si_3N_4/TiO_2 shell. In this study, the short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), power conversion efficiency (PCE) and fill factor (FF) are evaluated to determine the optoelectronic performance of the investigated NWs. Through comprehensive simulations, it has been demonstrated that the optimized structure significantly reduces optical losses and improves minority carrier transport, achieving a power efficiency of 22.487% with an enhancement of 49.74% over conventional truncated cone NWs. This innovative approach yielded a short circuit current density of 26.45 mA/cm^2, marking a significant advancement in radial junction NW solar cells.**

***Index Terms*—GaAs nanowire, III-V solar cell, heterojunction, Radial junction, Carrier-selective contacts**

I. Introduction

The development of efficient GaAs nanowire (NW) solar cells (SCs) has attracted significant attention in recent years due to their superior light absorption and potential for high efficiency [1]. By integrating carrier selective contacts, NW solar cells can achieve enhanced performance by reducing recombination losses and improving carrier collection. Recent studies have demonstrated the effectiveness of using materials such as indium tin oxide (ITO) and titanium dioxide (TiO_2) as carrier selective contacts to optimize device efficiency further [2]. For instance, the incorporation of an ITO/TiO_2 shell on GaAs NWs has been shown to significantly reduce optical losses and enhance short-circuit current density (J_{sc}) due to improved light management and reduced surface recombination. Moreover, advances in nanowire fabrication techniques and doping strategies have enabled precise control over the electronic properties of these hetero-structures, leading to power conversion efficiencies (PCE) that rival traditional planar solar cells [3]. This paper aims to explore the recent advancements in GaAs NW solar cells with carrier selective contacts, highlighting the impact of material selection, device architecture, and overall performance.

II. Simulation Methodology

Fig. 1(a) demonstrates a three-dimensional schematic of a Si_3N_4/TiO_2/GaAs NW core-shell heterojunction solar cell. The structure features an array with truncated cones (TC) at the top and cylinders at the bottom, conformally coated with TiO_2 and a layer of Si_3N_4 that functions as a transparent electric contact. Fig. 1(b) shows a detailed two-dimensional x-z cross-sectional view of a unit cell from our simulated structure, detailing the materials specification and their geometric properties. All Finite-Difference Time-Domain (FDTD) simulations were conducted using the commercially available Lumerical Device Suite. The GaAs NW diameter is denoted as d_{core} core, while the combined thickness of Si_3N_4 and TiO_2 is represented as T_{shell}. The periodic distance between adjacent NWs is denoted as "p". A three-dimensional FDTD method is employed to simulate light interaction with the solar cell unit cell. The unit cell is illuminated by a broadband, non-polarized plane wave source with a wavelength ranging from 300–1100 nm, incident perpendicularly on the GaAs substrate to mimic normal solar irradiation. To measure the light absorption within the unit cell, power monitors are positioned both above and below the cell in the simulation environment. The transmittance $\mathrm{T}(\lambda)$ and reflectance $\mathrm{R}(\lambda)$ spectra are obtained from the power monitors at each wavelength (λ). The light absorption $\mathrm{A}(\lambda)$ within the solar cell is then calculated using the formula: $A(\lambda) = 1 - R(\lambda) - T(\lambda)$.

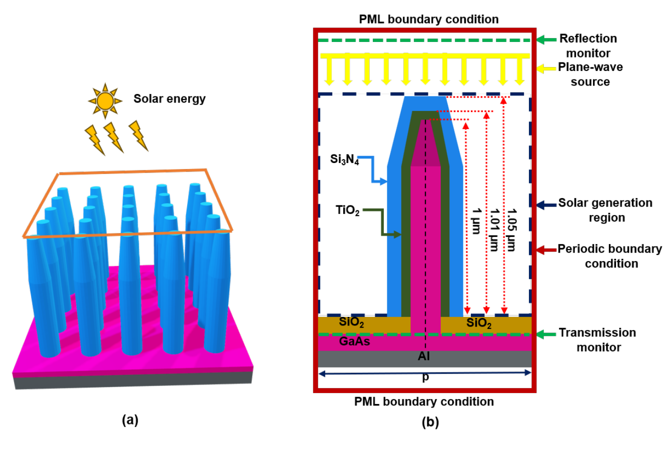

Fig. 1. Schematic of the solar cell: (a) 3-dimensional view of Si_3N_4/TiO_2/GaAs truncated cone nanowire array solar cell. (b) Simplified 2-dimensional structure used for simulating the solar cell optical properties in Lumerical software with design specifications.

III. Results and Discussions

In this work, we have optimized and fixed the height and diameters (top and bottom) of the truncated cone NW to 1 μm, 0.06 μm, and 0.12 μm, respectively. The TiO_2 conformal coating was fixed at 10 nm and varied the thickness of Si_3N_4 from 10 nm to 60 nm. To ensure low series resistance and a high short-circuit current density (J_{sc}), it is advisable to use a thicker Si_3N_4 shell. According to Fig. 2, for fixed d_{core}, optical J_{sc} increases significantly with the thickness of the outer shell (T_{shell}), reaching a maximum value of 28.94 mA/cm^2 at T_{shell} = 50 nm. The optical J_{sc} calculation was obtained using the formula: $J_{sc} = \frac{q}{hc} \int \lambda A(\lambda) I_{AM1.5G}(\lambda) d\lambda$. However, increasing the T_{shell} beyond 50 nm results in a decline in J_{sc} because a thicker photoactive material blocks more incoming light from reaching the core, hindering overall light absorption. The inclusion of a low-index Si_3N_4/TiO_2 shell around the truncated GaAs nanowires significantly diminishes optical losses and improves light trapping by improving the optical impedance matching between the air and the GaAs nanowires.

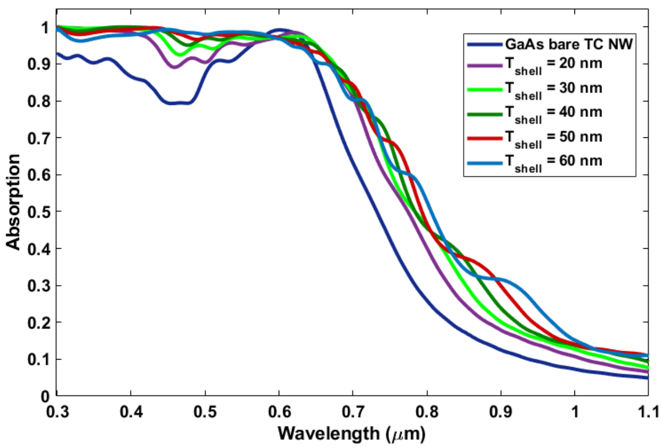

Fig. 2. Comparison of optical absorption in truncated cone NW arrays with and without Si_3N_4/TiO_2 shell thickness.

Fig. 3 illustrates a comparative J-V curve for radial and axial junction truncated cone GaAs NWs SCs. Table I further expands on this by presenting the photovoltaic parameters of our design alongside previously reported theoretical and experimental results for other nanowire-based solar cells. The results demonstrate that heterojunction SCs based on Si_3N_4/TiO_2/GaAs NWs can achieve an impressive J_{sc} of 26.45 mA/cm^2 and a high PCE of 22.487%. This highlights the potential of this design for high-performance solar cells

TABLE I
PERFORMANCE COMPARISON: OUR PROPOSED STRUCTURE VS. EXISTING RADIAL JUNCTION SCS (THEORY & EXPERIMENT)

Structures	J_{SC} **(mA/cm^2)**	V_{OC} **(V)**	***PCE* (%)**	***FF* (%)**
Si core-shell [4] (Theory)	18.45	0.920	11.60	74.6
GaAs p-i-n axial [5] (Experiment)	21.08	0.565	7.58	63.6
GaAs heterojunction [2] (Theory)	28.38	0.816	18.43	79.8
GaAs bare TC NW (**this work**)	18.54	0.991	15.01	81.7
GaAs heterojunction (**this work**)	26.45	0.990	22.48	85.8

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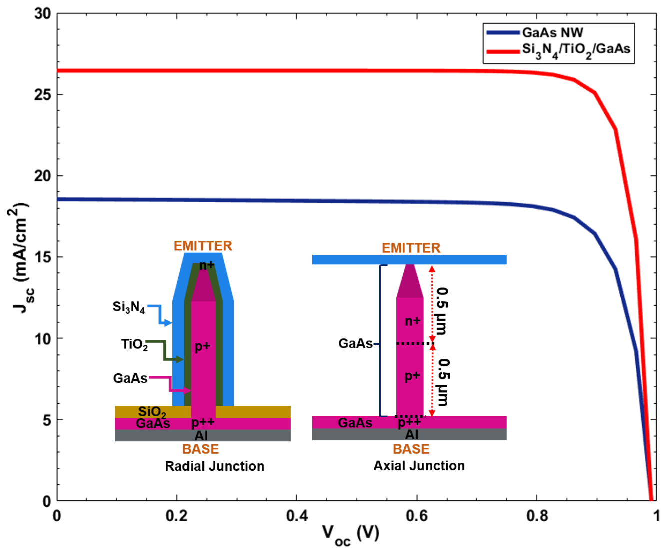

Fig. 3. The J-V characteristics of the optimized radial junction solar cell compared to an axial junction GaAs NW solar cell (inset: schematics of the simulated unit cells for both radial and axial junctions in Lumerical).

IV. CONCLUSION

This paper shows that the truncated cone NW-based radial p-n heterojunctions offer a promising route for creating highly efficient SCs. Optical simulations revealed that a strategically designed Si_3N_4/TiO_2 shell coating with a thickness of 50 nm on truncated cone GaAs nanowires can achieve a remarkable J_{sc} of 26.45 mA/cm^2 and a broad light absorption of 73%. Beyond optimizing light capture, we further investigated how core doping at the TiO_2/GaAs interface influence the cell performance. Our analysis suggests that a p-type core doping concentration of $1{\times}10^{18}$ cm^{-3} is ideal for achieving a PCE of 22.487%. This translates to a J_{sc} of 26.45 mA/cm^2, a V_{oc} of 0.9907 V, and a FF of 85.8%. In essence, this study paves the way for a new generation of SCs that are more efficient and potentially easier to manufacture.

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