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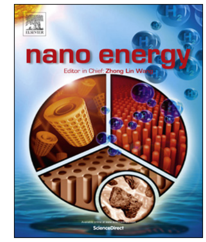

RAPID COMMUNICATION

Improved optical absorption of silicon single-nanowire solar cells by off-axial core/shell design

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Abstract
Single-nanowire solar cells (SNSCs) are attracting increasing interest due to their unique antenna-effect-mediated light-trapping and the efficient charge separation through thin semiconductor junctions. However, for such newly emerging photovoltaic devices, the optical and photoconversion performance is still far from the expectation. More effective strategies which are capable of providing broadband/high absorption and high electrical outcome are strongly desired. In this study, we introduce the concept of symmetry-breaking into the core/shell silicon SNSCs, which enables a substantially enhanced optical absorption under an improved coupling between the photoactive material and the focus of the dielectric shell. By properly deviating the silicon core away from the dielectric shell center (i.e., the off-axial core/shell design), the light-trapping capability of the device is significantly improved in almost the whole spectral band without degrading the carrier collection performance. Our optoelectronic simulation exhibits that the photocurrent density as well as the light-conversion efficiency of free-standing SNSCs can be doubled (enhanced by ~40%) compared to that of the system under bare (co-axial core/shell) nanowire design; moreover, the device performance under such asymmetric design can be further improved with introducing the metal-coated substrate.

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Introduction

Single-nanowire solar cells (SNSCs) have recently attracted considerable attention for advantages over their planar counterparts, such as the extreme light-trapping capability, the efficient carrier transport, and the deep-subwavelength device scale which is highly suitable for integration into chips [1-15]. Besides the photovoltaics, single nanowires (NWs) can find much broader applications, e.g., the optical waveguides for strong light confinement [16], photodetectors with high responsivity [17], and lasers with an active nanowire cavity [18].

In 2007, the first silicon SNSC was fabricated with the maximum output power (conversion efficiency) of 200 pW (3.4%), revealing the possibility of this kind of compact photovoltaic cell to serve as the integrated power source for optoelectronic nanosystems [1]. For photovoltaic applications, excellence in broadband light-harvesting is the first and very crucial step, which normally appeals to the advanced light-trapping strategies. For SNSCs, precisely controlling the size and cross-sectional morphologies of NWs has been proved to be an efficient way [9-11]; among various designs, the transparent dielectric nano-shell has usually been employed to exhibit both optical and electrical benefits [12-14]. For example, we presented that the nano-shelled rectangular gallium arsenide (GaAs) SNSCs can provide light absorption and external quantum efficiency (EQE) over 100% under both transverse electric and magnetic (TE and TM) incidences [12]. For coaxial heterogeneous GaAs SNSCs, the nano-shell and window layers can assist lowering the photocurrent loss due to surface carrier recombination [13]. For the optimally designed co-axial c-Si/a-Si (crystalline silicon/amorphous silicon) SNSCs, the photocurrent can be enhanced by ~60% by coating the non-absorbing dielectric shell [14].

However, the existing designs on core/shell SNSCs are mostly based on the conventional symmetric (co-axial) configurations. As indicated that the upper limit of light-trapping in one-dimensional symmetric grating structures is only half of the asymmetric ones when the periodicity is comparable to the wavelength [19,20]. Our recent study also showed that the omnidirectional absorption enhancement can be obtained in the symmetry-broken rear-crescent-deformed SNSCs benefited from the significantly enhanced nanocavity resonances [15]. These indicate that the asymmetric configuration might be an efficient way to further improve the light-harvesting performance of SNSCs. In this study, we report an off-axial core/shell design for silicon SNSCs, in which the photoactive region is deviated properly from the shell center. The asymmetrical modification to the system leads to dramatically improved light absorption in a broad spectral band. The detailed analysis of the electric field and power flow distributions shows that the enhancement arises mainly from the strengthened nanofocusing effect under an improved coupling between the photoactive material and the focus of the dielectric shell. The finite-element method (FEM) simulations indicate that the photocurrent can be improved by 116% and 40% relative to the bare (without the shell) and co-axial core/shell SNSCs, respectively. In addition, the superior light-harvesting capability can be sustained in a wide range of incident angles. Further electrical simulation by addressing the detailed carrier transport and recombination process shows that an enhancement ratio of 42% in light-conversion efficiency over the conventional symmetric co-axial configuration can be achieved. An extended study validates the capability of achieving further improved optical and electrical performance with incorporating a back metallic reflector to the designed off-axial Si SNSCs.

Model and methods

The cross-sectional configurations of the bare, co-axial and off-coaxial Si (core)/SiO_2 (shell) SNSCs are schematically shown in the insets of Fig. 1. The characterized geometrical parameters are the core radius r (200 nm), the shell thickness s and the offset distance d of the core from the shell center [i.e., $d>0$ (<0) for upward (downward) offset]. Based on the optical constants from Palik [21], the FEM-based full-wave electromagnetic calculations are performed [22]. The length of nanowire is assumed to be far beyond the diameter, allowing the use of two-dimensional (2D) simulation [5,13]. The absorption efficiency (Q_{abs}) is defined as the ratio of the absorption cross section to the geometrical cross section [10,14]. The unpolarized illumination is represented by the average of TE (electric field parallel to the axis) and TM (electric field perpendicular to the axis) incidences, i.e. $Q_{abs} = (Q_{abs}^{TE} + Q_{abs}^{TM})/2$. The

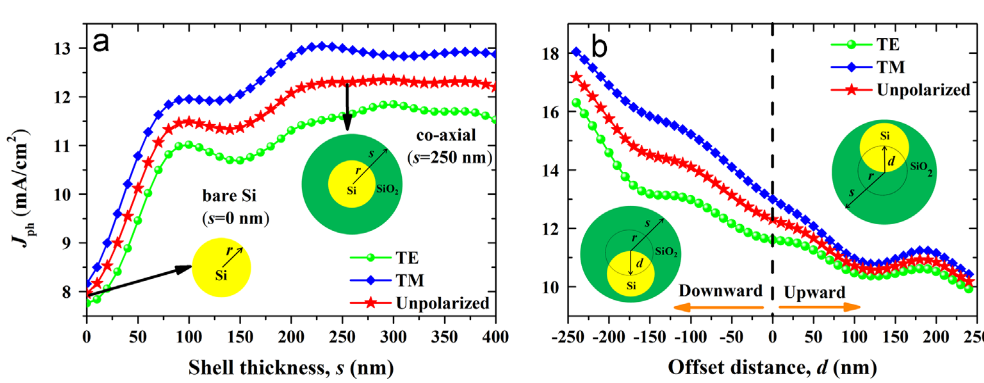

Fig. 1 J_{ph} versus (a) the shell thickness s of the co-axial and (b) the offset distance d of the off-axial SNSCs for TE, TM and unpolarized normal incidences. The insets are the corresponding schematic diagrams.