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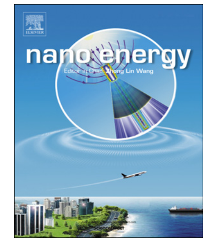

RAPID COMMUNICATION

Broadband light-concentration with near-surface distribution by silver capped silicon nanowire for high-performance solar cells

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Abstract
Silicon nanowire (SiNW) shows striking light-concentration ability and thus holds promising application potentials in photonic devices. However, its narrow working waveband strongly affects its performance over the entire visible spectrum. Here, a silver capped SiNW structure (Ag-cap/SiNW) is presented to broaden the working waveband of the pure SiNW. Discrete dipole approximation simulations show that, by this structure, the light-concentration waveband can be significantly broadened from 440–620 nm (pure SiNW) to 300–620 nm. Thus, using the Ag-cap/SiNW in the solar cell, the ideal photocurrent density can be enhanced 16% compared with that using pure SiNW. Furthermore, the concentrated light shows the feature of the strong near-surface distribution around the Ag-cap/SiNW. This distribution feature gives a reasonable explanation for the huge superiority of the radial junction SiNW solar cells to axial junction SiNW solar cells from optical aspect. Additionally, due to the intrinsic waveguide property of SiNW, this Ag-cap/SiNW also has great potential applications in photonic devices such as nanoscale optical biosensors and light-integrated-chips.

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Introduction

Silicon nanowire (SiNW) is attracting an increasing interest in recent years [1-6]. Among other excellent properties, its unique optical properties, the ability to capture and concentrate light with regional transverse distribution at nanoscale [7-11] makes it hold promise for potential applications as nanoscale building blocks in photonic devices: SiNW based solar cells [12-15], sunlight-driven solar water splitting [16], nanoelectronic power sources [17,18], photoelectrochemical cell [1,19], photodetectors [20,21], and even the fascinating light-integrated-chip [22].

The main drawback of using SiNW as light concentrator is that it only works at various narrow wavebands [11,23,24], which correspond to the resonance wavelengths of the lowest-order leaky mode supported by the SiNW [25,26]. These narrow working wavebands strongly limit its performance over the entire visible spectrum, and thus limit its practical application in some fields. For instance, in photovoltaic cells [13-15,17,27] and photoelectrochemical cells [1], broadband light-concentration is of great concern to ensure maximum utilization of the sunlight to generate high photocurrent. In sunlight-driven solar water splitting [16], a broader light-concentration waveband is also very helpful to achieve higher splitting efficiency by generating more photogenerated carries.

Fortunately, silver nanoparticle also possesses outstanding light-concentration function [28-30] due to the plasmonic effect, and at the same time its working waveband is rightly complementary with that of the SiNW. So, combining the silver nanoparticle and the SiNW together as a composite structure should be one possible way to avoid the limitation of the SiNW in broadband light-concentration.

To date, only few works on silver-nanoparticle/SiNW composite structure has been reported [23,31,32], and the broadband light-concentration ability hasn't been realized in all of them. For instance, in Ref. [31] where a silver nanoparticles decorated SiNW structure was presented, only the light-concentration ability of the silver nanoparticles (about 50-fold) was highlighted but that of the SiNW was almost vanished. We think that the failure of the silver nanoparticles decorated SiNW in broadband light- concentration is mainly due to the high density of the silver nanoparticles, which wholly shield the light-concentration function of the SiNW by abundant geometrical scatterings.

So, in this work, a silver nanoparticle capped SiNW structure (Ag-cap/SiNW) is designed to realize the broadband light-concentration function. The single silver cap (Ag-cap) can only cover a small geometrical area, thus will not affect the light-concentration ability of the SiNW significantly. Besides, in this Ag-cap/SiNW structure, the concentrated light could be further expected to distribute regionally in transverse direction as that in the pure SiNW [7-11]. This is because the light concentrated by the Ag-cap has great tendency to be unidirectionally scattered into the SiNW, thus to be coupled into the guided modes following their field distribution. This regional transverse distribution is of great importance in photonic devices optimization [7]. In a word, by the Ag-cap/SiNW, a broadband light-concentration function with regional transverse distribution is expected to be realized.

Based on discrete dipole approximation (DDA) method [33-35], the optical properties of the Ag-cap/SiNW are investigated in detail. The two expected light-concentration functions are both realized. The light-concentration waveband is broadened from 440-620 nm (pure SiNW) to 300-620 nm, which brings a 16% enhancement of ideal photocurrent density in solar cell using the Ag-cap/SiNW compared with that using the pure SiNW. The concentrated light distributes regionally in transverse direction, and thus shows a feature of the strong near-surface distribution within and out the silicon part. This provides reasonable optical explanation for the superiority of radial junction to axial junction SiNW solar cells. Such insight is essential to the design and optimization of the efficient solar cells and other optical devices.

Model, simulation method and reliability testing

A schematic diagram of the presented Ag-cap/SiNW is shown in Fig. 1**a**. The Ag-cap is designed with hemispherical end for easily preparing [36]. The size parameters are set referring to the reported well performed SiNW solar cells. The diameter is set to 80 nm, which corresponds to the optimized light-trapping effect [37]. The total length is set to 3.0 μm, which approximates to the average of the values, 1.5 to 4 μm [37,38], for optimized conversion efficiency. To make the light-concentration effect of the Ag-cap remarkable (see the Supporting Information), its length is set as 0.7 μm. Since the diameter is large enough, the quantum confinement effect [13,39] is neglected and thus the complex dielectric constants of bulk silver and silicon, as shown in Fig. 1b and c, are used [40,41]. Besides, only the incident light from the Ag-cap is considered as the light-trapping effect of SiNW is insensitive to the incident angle [24].

The extinction, scattering and absorption spectra of the Ag-cap/SiNW, as well as the light filed distribution within it are calculated using the DDA method by code DDSCAT 7.3 [33]. Firstly, the Ag-cap/SiNW is replaced by an array of point dipoles, located on cubic lattices. Then, the electromagnetic scattering problem of the incident light interacting with this point dipoles array is solved. Finally, the spectrum and light field distribution properties are derived. A frame description of the DDA method is given as follows.

Let the index $j=1,\ldots N$ run over the occupied lattice sites. Each dipole j is characterized by a polarizability tensor α_j, Such that $\vec{P}_j=\alpha_j\vec{E}_{\text{ext},j}$, where $\vec{P}_j$ is the instantaneous dipole moment of dipole j, and $\vec{E}_{\text{ext},j}$ is the instantaneous electric field at position j due to the incident light on the dipole plus the other $N-1$ oscillating dipoles. The key problem in DDA is to obtain a self-consistent set of dipole moments $\vec{P}_j$. $\vec{P}_j=\alpha_j\vec{E}_{\text{ext},j}$ can be rewritten as N simultaneous complex vector equation of the form

$$\vec{P}_j=\alpha_j(\vec{E}_{\text{inc},j}-\sum_{k\neq j}A_{jk}\vec{P}_k) \tag{1}$$

where $\vec{E}_{inc,j}$ is the electric field at position j due to the incident light, and $-A_{jk}\vec{P}_k$ is the contribution to the electric field at position j due to the dipole at position k.

$$\vec{E}_{\text{inc},j}=\vec{E}_0\exp(i\vec{k}\cdot\vec{r}_j-i\omega t) \tag{2}$$