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Ying Wang(王莹), Xin-Hua Li(李新化)
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Light trapping and optical absorption enhancement in vertical semiconductor Si/SiO_2 nanowire arrays*

Ying Wang(王莹)[1] and Xin-Hua Li(李新化)[2,3,†]

[1] College of Electrical Engineering and Automation, Anhui University, Hefei 230601, China
[2] Key Laboratory of Material Physics, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei 230031, China
[3] Yuhuan Scientific and Technological Transformation Center, Chinese Academy of Sciences, Taizhou 317600, China

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The full potential of optical absorption property must be further cultivated before silicon (Si) semiconductor nanowire (NW) arrays become available for mainstream applications in optoelectronic devices. In this paper, we demonstrate both experimentally and theoretically that an SiO_2 coating can substantially improve the absorption of light in Si NW arrays. When the transparent SiO_2 shell is coated on the outer layer of Si NW, the incident light penetrates better into the absorbing NW core. We provide the detailed theoretical analysis by a combination of finite-difference time-domain (FDTD) analysis. It is demonstrated that increasing the thickness of the dielectric shell, we achieve 1.72 times stronger absorption in the NWs than in uncoated NWs.

Keywords: nanowire, nanosphere lithography, finite-difference time-domain (FDTD)

PACS: 61.46.Km, 71.35.Cc, 61.46.–w **DOI:** 10.1088/1674-1056/27/2/026102

1. Introduction

Recently, intensive attention has been paid to the silicon (Si) semiconductor nanowire arrays (NWAs), due to their potential applications in low cost and high power conversion efficiency photovoltaic devices. Compared with conventional planar thin-film structure, the NWAs have been proved to have many advantages in integrating the NWA structure into the photo-electrical devices. By combining light trapping effects, nanowires (NWs) can enhance the light absorption with reducing the material used.[1] Meanwhile, as arranged in the coaxial p-n structure, the NWA facilitates carrier collection and makes the photo-electrical devices less sensitive to the defect concentration in the semiconductor material.[2,3]

Till now, intensive work has demonstrated that silicon (Si) NWAs exhibit excellent light absorption, particularly in the short wavelength region. But to maintain high absorption, high filling ratio for NW arrays is required.[4] After introducing these high filling ratio Si nanostructures, conformal deposition of the transparent electrodes over the nanostructure surface becomes a challenge.[5] These factors increase the complexity and manufacturing cost of device fabrication.

To tackle this issue, in this report we fabricate diluted Si NW by metal-assisted chemical etching (MACE). To increase the absorption of the Si NW, we add a transparent SiO_2 coating to the outer layer of Si NW. We demonstrate experimentally and theoretically that the transparent dielectric coating can be used for strongly enhancing absorption in the core Si NWs for a broad wavelength range. Furthermore, at the optimized thickness of the dielectric shell, the strong light absorption in the NWs can be achieved to be more than 1.7 times that in the completely uncoated Si NWs. Hence, the addition of the transparent SiO_2 shell over the Si NW can reduce the complexity and manufacturing cost, which is greatly useful in guiding the design and fabrication of high-efficiency low-cost Si NW array solar cells.

2. Methods

For the experimental investigations, we obtain the ordered arrays of Si NWs by the nanosphere lithography (NSL) assisted MACE.[6–8] The substrates used in this study were n-type Si (100) ($\rho \sim 3\ \Omega$·cm). After the Si substrates were degreased by ultrasonic cleaning in acetone, polystyrene (PS) colloidal sphere monolayer was prepared by gas/liquid interface self-assembly method. The original diameters of PS spheres were 500 nm. After that, the Si substrate with PS sphere template was transported into the reactive ion etching (RIE) region. By an anisotropic etching under an oxygen (O_2) flow rate of 16.5 sccm, a pressure of 2.0 Pa, and an RF power of 100 W, the diameter of PS sphere was reduced. Then, a Ti(2 nm)/Au(25 nm) bilayer film was prepared onto the Si substrate by thermal evaporation. Subsequently, the PS sphere was removed from the substrate by ultra-sonication in toluene and the ordered catalytic metal meshes were formed. Then Si NWAs were prepared by MACE in a mixture of

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†Corresponding author. E-mail: xinhuali@issp.ac.cn
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etching solution (10:2:10, v/v/v, HF/H_2O_2/ H_2O). The SiO_2 layer was deposited onto the outer surface of the prepared Si NW at 300 °C, and onto the NWs by atomic layer deposition (ALD). The morphology of the prepared Si NWAs with SiO_2 shell is shown in Fig. 1(a). The broadband optical reflection measurements were performed in a wavelength range of 400 nm$< \lambda <$ 1000 nm via a Zeiss optical microscope equipped with an optical probe. In the measurements, the unpolarized light was focused on a sample by a 20× objective. The focused square spot has an area of 20 μm×20 μm. The reflection light was collected with the same objective lens and detected by a spectrometer. The theoretical study of the optical response of SiNWs was performed through electromagnetic simulation by using the finite-difference time-domain (FDTD) method, which has been presented in detail elsewhere. The three-dimensional (3D) optical simulations were carried out by using the software package FDTD Solutions (Lumerical, Inc.). A hexagonally arranged column array was proposed as the unit cell to model the periodic Si NW as fabricated by MACE (Fig. 1(b)). The complex refractive indices used to describe the optical property of materials (i.e., SiO_2, Si) in this simulation are taken from the Ioffe n & k Database.[9]

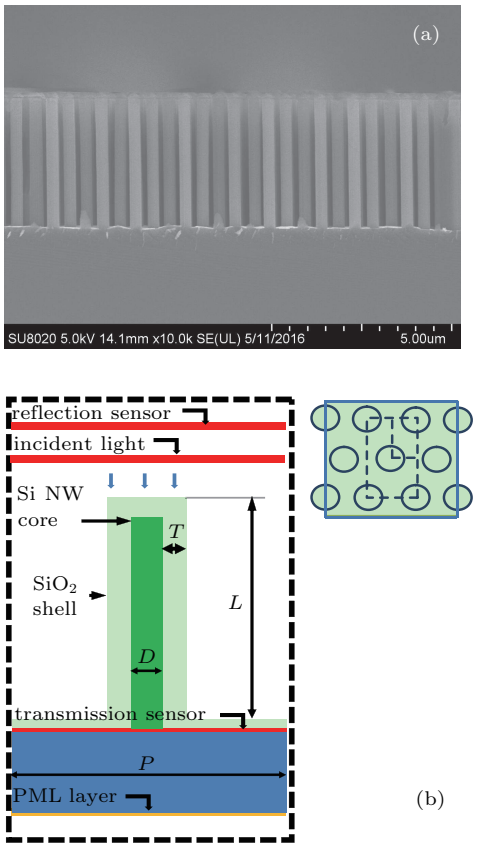


Fig. 1. (color online) (a) SEM morphology of Si/SiO_2 nanowire array with core–shell structure. (b) Schematic diagram and simulated unit of core–shell Si/SiO_2 NW array modeled in this study. In this simulation, geometric parameters are selected as follows: diameter (D) of Si NW = 100 nm, length (L) of NW = 5000 nm, period (P) = 500 nm by varying the SiO_2 thickness.

3. Results and discussion

In marked contrast to the gray color of bulk silicon, a clear color change can be observed in the samples with the bare and coated NW array respectively as seen in the insets in Fig. 2(a). We demonstrate that the bare Si nanowires take on a mazarine color, in marked contrast to the gray color of bulk silicon. This implies that the light propagations in the Si NW array are very different from those in the planar Si structure. As the conformal SiO_2 coating is prepared onto the outer layer of the Si NW, the NW array shows a dark color, which implies less reflection of the NW array with this structure.

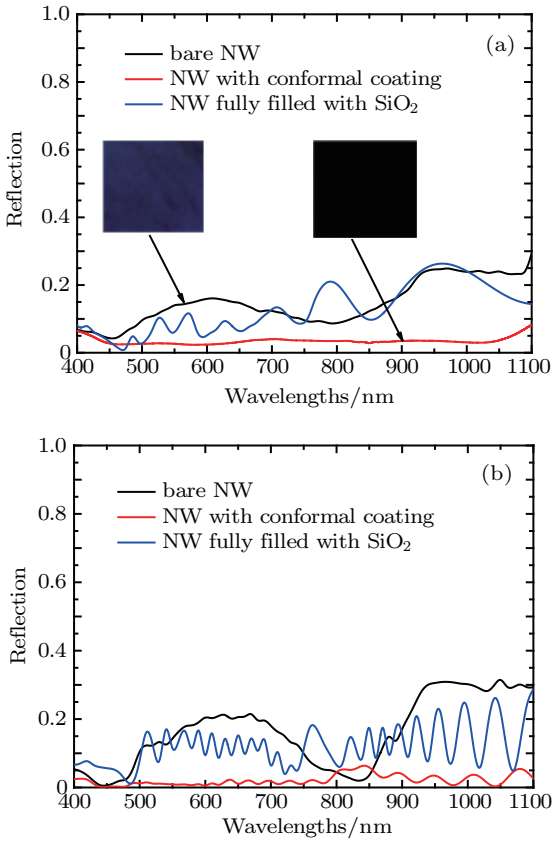


Fig. 2. (color online) (a) Measured reflection spectra of an Si NW array of period P = 500 nm and NW diameter D of core = 160 nm and length L = 5000 nm for the Si NW arrays with different SiO_2 shells. The two colorful inset squares are optical images of the NW array in the cases without and with 60-nm conformal SiO_2 coating. (b) Calculated reflectance spectra as a function of the SiO_2 coating thickness for the same geometries as that in panel (a) obtained by FDTD simulations.

To elucidate the mechanisms behind the observed phenomenon, we measure the reflectance spectra as a function of wavelength λ for the Si NW array coated with SiO_2 layers with various coating thickness values. For the bare Si NW arrays, the reflection spectrum features two broad dips between 600 nm–900 nm and 400 nm–500 nm and a reflection oscillation above 700 nm. As the 60-nm conformal SiO_2 shell is prepared, the measured optical reflectance is much lower than that from normal Si film for all wavelengths investigated. Furthermore, the overall trend of the reflectance of the NW array is reduced as the SiO_2 coating is added. Hence the addition

of the transparent shell has the potential to adjust the optical response in optoelectronic applications. As the NW is fully filled with the transparent SiO_2, the overall reflection increases again and some reflection oscillations can be observed in the reflection spectrum.

To accurately analyze the optical response, especially the absorption of the three-dimensional (3D) Si NW array system, we use numerical simulations based on the FDTD method to solve Maxwell's equations. Figure 2(b) shows the simulated reflectance as a function of wavelength λ for NW array with the same geometrical parameters as those in the experiments. We obtain very good agreement between the measured and modeled spectra. The simulated optical response of the NW array reproduces very well both the magnitude of the reduced reflectance and the red shifts of the spectra under different coating conditions.

From the reflection spectrum of NW, only limited information correlated with the structure and the optical property of NW can be obtained. To further understand the optical response of the Si/SiO_2 core-shell structure, the absorption variations with the shell thickness need further investigating. By employing energy balance, the absorption A of the NWs can be obtained from $A = 1 - R - T$, where R is the reflectance of the NW array and T is the transmittance into the Si substrate.[10,11] Figure 3(a) shows the absorption (of the NWs) variations with the thickness of the conformal non-absorbing SiO_2 shell. Most importantly, near the wavelength of 800 nm, absorption peaks can be observed. The absorption peaks are indeed due to a coupling of incident light into HE_{1n} guided modes supported in the nanowires. Besides this, one can find that the absorption in Si NW increases substantially, as a 60-nm thick SiO_2 shell is added. At the wavelength of 880 nm the absorption is enhanced by more than 172%. It is interesting to note that the absorption enhancement is obtained in the case without changing the size or shape of the absorbing Si core of the NWs.

In order to understand the propagation of incident light in the NWA, we calculate the generation rate within the array from

$$G_{\text{opt}} = \frac{\text{real}(\nabla \cdot S)}{2\hbar\omega} = \frac{\varepsilon'' |E|^2}{2\hbar}, \tag{1}$$

where ε'' is the imaginary part of the complex permittivity and E is the electric field.[12–14] We obtain the generation rate for the uncoated Si NW and 60-nm-thick SiO_2-layer coated Si NWs at three typical wavelengths. As plotted in Fig. 3(b), the photogeneration rates at an incident wavelength of 400 nm are concentrated near the top and side of the nanowire for both structures. When the incident wavelength is increased to 600 nm, one can find that the optical generation exhibits more homogeneously spreading over the uncoated Si NWs. Meanwhile, a small fraction of the incident wave is transmitted to the substrate. In contrast, the optical generation for NWs with 60-nm SiO_2 coating is enhanced in the core Si NW. This result accords well with the absorption enhancement of core-shell Si/SiO_2 NW system as shown in Fig. 3(a). At 800 nm, the photogeneration rates are concentrated to several lobes that form along the uncoated and SiO_2 layer coated Si NW, indicating strong guided modes confined inside the NWs. By comparison, more intensive photogeneration rate can be observed in Si NW with 60-nm inorganic coating than that in the uncoated Si NW. This result accords well with absorption curve shown in Fig. 3(a). To quantitatively study the absorption enhancement

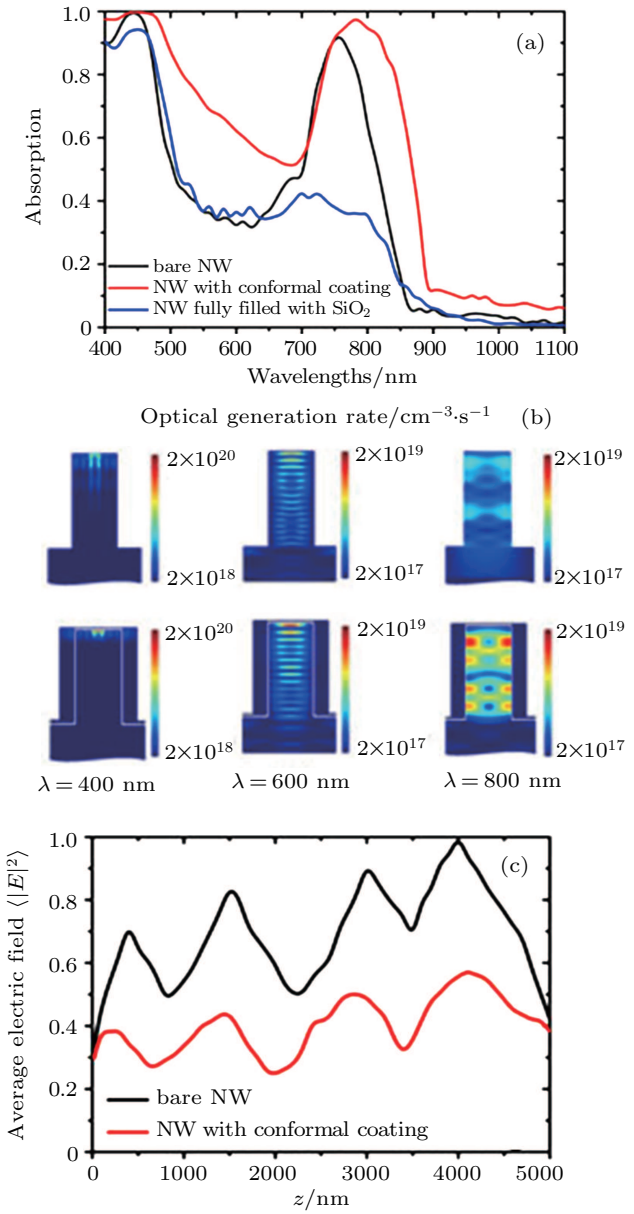


Fig. 3. (color online) (a) FDTD simulation absorptions versus wavelength for the bare Si NW arrays (black solid line) and Si NW arrays with 80-nm SiO_2 shell (red solid line). (b) Optical generation rates for uncoated Si NWA and 60-nm-thick SiO_2-layer coated Si NWA at three typical wavelengths: 400, 600, and 800 nm. (c) Average electric field $\langle |E|^2 \rangle$ as a function of axial position (Z, where the bottom of Si NW is set to be the zero point) of the NW ($\langle |E|^2 \rangle$ is normalized to the maximum value in the Si/SiO_2 (60 nm) structure).

at the incident wavelength of 800 nm, we calculate the average electric field $\langle|E|^2\rangle$ in the core Si NW as a function of axial position (Z) along the NW axis. As shown in Fig. 2(b), the average electric fields $\langle|E|^2\rangle$ for both uncoated Si NW and 60-nm-thick SiO_2-layer coated NW are obtained. The mean value of the electric field inside the uncoated NWs is $\langle|E|^2\rangle = 0.376$ (calculated as the average of $\langle|E|^2\rangle$ over Z). For the 60-nm-thick SiO_2-layer coated NWs, $\langle|E|^2\rangle = 0.652$. Hence, the 60-nm transparent SiO_2 coating causes a value 1.73 larger than $\langle|E|^2\rangle$ inside the Si NW, which is close to the absorption enhancement at this wavelength as shown in Fig. 3(a). Obviously, the non-absorbing dielectric SiO_2 shell can drastically increase the absorption in vertical semiconductor NWAs.

From the above discussion, it is clear that the absorption of NWA is significantly enhanced by the introduction of the transparent SiO_2 coating. But for NWA structure, the light absorption of the Si/SiO_2 NWA with core–shell structure is quite sensitive to structural parameters. To determine an optimized geometric configuration, we calculate the ultimate photocurrents for various organic coating thickness values from the following equation, on the assumption that all photogenerated carriers can contribute to photocurrent:

$$J_{\rm ph} = (e/hc)\int \lambda A(\lambda) I(\lambda)\,{\rm d}\lambda, \tag{2}$$

where e is the elementary charge, h is the Planck's constant, c is the light speed, $I(\lambda)$ is the AM1.5G spectrum, and $A(\lambda)$ is the absorption of the NW array.[15,16] The ultimate photocurrents as a function of the fill factor for different diameters are shown in Fig. 4.

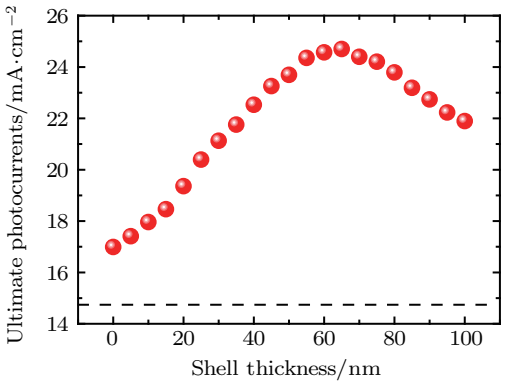


Fig. 4. (color online) Ultimate photocurrent of the Si/SiO_2 NWA as a function of SiO_2 coating thickness. Dashed line indicates the ultimate photocurrent for Si NWA fully filled with SiO_2.

For the 160-nm Si NW coated with SiO_2 shell, the ultimate photocurrent first increases with transparent coating thickness increasing, then reaches a maximum value of $\sim$ 24.6 mA/cm^2 at an SiO_2 shell thickness of 60 nm. Note that at this coating thickness, the photocurrent is enhanced by a factor of 1.39 when adding the 60-nm thick shell. Obviously, much improved light absorption could be obtained, when transparent shell with an appropriate thickness is coated on the photoactive Si NWs. The further increase of the SiO_2 shell thickness causes the ultimate photocurrent to decrease gradually. One can see that the ultimate photocurrent of Si NW with fully filled SiO_2 is about 9.9 mA/cm^2 lower than that with the conformal coating condition of 60 nm. The reduction of ultimate photocurrents can be attributed to the increased reflection, as the Si NW array is fully filled with SiO_2. This shows the superiority performance of core-shell structure as compared with fully filled condition.

4. Conclusions

In this work, an optical simulation is conducted to optimize the optical characteristics of Si NWA with transparent SiO_2 shell. It is found that the introduction of conformed transparent SiO_2 coating on Si NWA can further increase the absorption of photoactive inner Si NWA. At an optimized size, the proposed core-shell NWA structure exhibits the promising ability to absorb photos. Furthermore, Si NWs combined with a transparent SiO_2 shell yield surface defect passivation effects besides exhibiting a substantial absorption enhancement. In the fabrication of PV device, the use of Si NW with low filling factors can reduce the complexity and manufacturing cost, which is greatly useful in guiding the design and fabrication of high-efficiency, low-cost, Si NW array solar cells.

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