Method to determine the optimal silicon nanowire length for photovoltaic devices

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The length of the silicon nanowire (SiNW) is a key parameter in photovoltaic devices, as it dramatically decides the light-harvesting and carrier recombination. Here, we develop a method to determine the optimal SiNW length for photovoltaic devices, by comparing the light-harvesting efficiency of SiNWs with various lengths. The light-harvesting efficiency is measured by the light intensity in the SiNW, and the fraction of the length with high light intensity in its whole length. Under these criteria, we find that the optimal SiNW length is around 3 μm. This method is helpful in further optimization and application of SiNW-based solar cells. © *2015 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4914372]

Silicon nanowire (SiNW) based solar cells hold great promise for third-generation photovoltaics and for powering nanoscale devices.[1–4] Since the fabrication of nanowire arrays, these solar cells will become cheaper and more efficient than the corresponding bulk devices. Besides, the SiNW array is also beneficial for the strain relaxation[5] thus provides great freedom in new device structure designs. However, as of today, the highest efficiency of the SiNW solar cell, 17.11%,[6] is still far from the theoretical limited efficiency 29.8%.[7] To enhance the conversion efficiency, there are two fundamental ways from the optical and electrical viewpoints: to enhance the incident light entering the device and to suppress the carrier recombination. Fall on the SiNW solar cell system, the light-harvesting depends on the geometry design (including diameter[8–10] and length[11–13]) of the SiNW, while the carrier recombination merely depends on the length of SiNW as the carriers are easily trapped by surface defects during their axial transmission process.[14,15] So, diameter and length of the SiNW are the two key size parameters in determining the performances of SiNW solar cells. The SiNW diameter has been demonstrated to have an optimal value 80 nm,[11] so that the resonance wavelength of SiNW with this diameter rightly corresponds to the highest energy density in the sunlight spectrum (AM1.5d ASTM G173–03). However, the optimal SiNW length cannot be determined so simply, since an improved light-harvesting and a reduced charge recombination are two conflicting goals.[16] Using electron-beam-induced current microscopy, Allen *et al.*[17] have found that the minority carrier diffusion length in SiNW with 80 nm diameter is only about 100 nm, 1/100 of that in bulk. This results in that the carrier recombination loss is the main limitation for the conversion efficiency of SiNW-based solar cells.[6,14,15] Therefore, it dramatically requires that the SiNW with optimal length has the most effective light-harvesting efficiency (LHE), to minimize the carrier recombination as much as possible. In this work, based on theoretical simulations, we propose the criteria to measure the light-harvesting efficiency of SiNW, and develop a method to determine the optimal SiNW length by comparing the LHE of SiNWs with various lengths. The criteria are extracted from the intensity variation profiles of light propagating in the SiNW. The obtained optimal SiNW length, around 3 μm, locates at the length range of 2–5 μm,[16] in SiNW with which the enhanced light-harvesting can dominate over carrier recombination. These insights are helpful in further optimization of SiNW-based solar cells.

We model the SiNW as circular cylinder with a hemisphere top to represent the actual shape, as shown in Fig. 1(a). The diameter is set to 80 nm, and the length varies from 2 μm to 6 μm. Since the light-trapping effect of SiNW is insensitive to the incident angle,[10] only the incident light with y-polarization irradiating from the top is considered. The complex dielectric constants of bulk silicon are used,[18] because the SiNW is large enough to neglect the quantum confinement effect.[14] We carry out simulations employing the discrete dipole approximation (DDA) method with code DDSCAT 7.3,[19] whose reliability has been carefully tested. On a silicon sphere with 80 nm diameter, as shown in Fig. 1(b), the simulated extinction efficiency curve is excellent consistent with that derived from the rigorous Mie theory.[20] On the SiNW with 70 nm diameter and 2.6 μm length, as shown in Fig. 1(c), the locations of the valley and peak in the simulated extinction efficiency curve coincide perfectly with the peak and valley in the measured reflectance spectrum of a SiNW array, respectively. These calculations fully confirm the reliability of the DDA method on investigating the optical properties of silicon nanostructure.

As the start, we carry out simulations on a SiNW with the length of 3 μm to establish the criteria in measuring the LHE. Fig. 2(a) shows the obtained absorption efficiency curve of it. Clearly, the resonance wavelength of this SiNW is 524 nm, which rightly corresponds to the highest energy density in the sunlight spectrum (AM1.5d ASTM G173–03). In addition, the absorption efficiency at this wavelength reaches about 136, which indicates the SiNW has excellent

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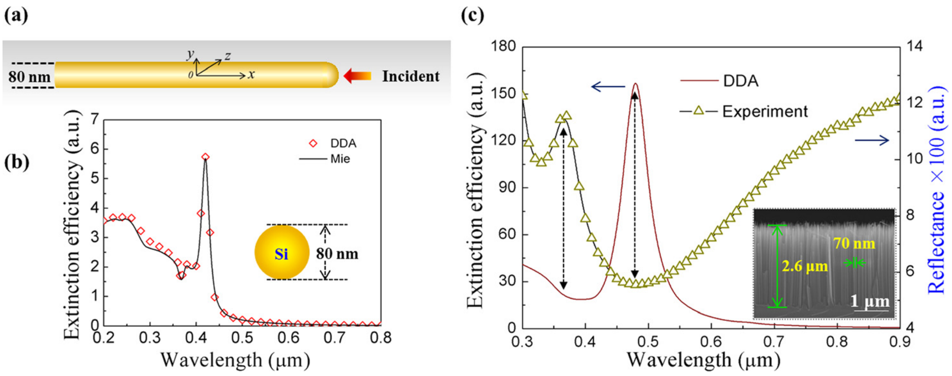

FIG. 1. (a) Schematic of the SiNW geometry and the excitation scheme. Comparison of the simulated extinction efficiency curve of (b) silicon sphere with that derived from Mie theory and (c) a SiNW with the measured reflectance spectrum of a corresponding nanowire array.

light-absorption ability. Such results denote that 524 nm is a wavelength of representative significance in investigating the LHE of the SiNW. Therefore, the criteria for the SiNW's LHE are presented under this wavelength.

Since the light absorption amount is proportion to light intensity, which is equal to the square of electric field intensity ($|E|$), the maps of the electric field distribution within the SiNW, as shown in Fig. 2(b), can intuitively reflect the local light-harvesting ability in the SiNW. From the vertical section, we can see that, along the SiNW, the filed intensity exhibits a strange first increasing and then decreasing trend. This denotes that there is quite a long distance in the SiNW, where the local light-harvesting amount maintains high level. To describe this feature quantitatively, we extract the $|E|$ values along the SiNW from a representative line, whose projection corresponds to the maximum field intensity in the cross section (marked as point O). Then, we take the extracted $|E|$ values squared and plot $|E|^2/|E_0|^2$ versus x in Fig. 3. Where $|E_0| = 1$, is the field intensity of the incident light.

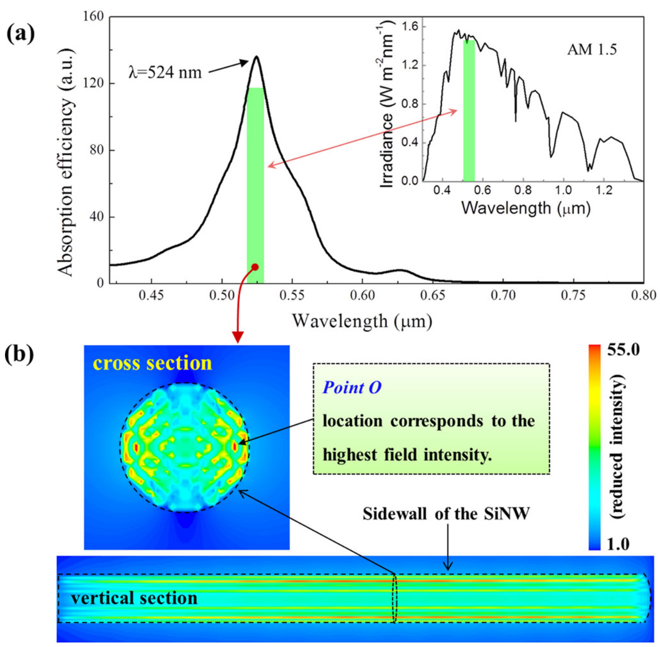

FIG. 2. (a) The absorption efficiency curves of a SiNW with 3 μm length. Inset: the irradiance of the AM 1.5 spectrum. (b) The reduced electric field distribution in and around the SiNW, including a cross and a vertical section. Point O denotes the location corresponding to the highest field intensity. The z-axis and x-axis ratio in the lateral direction of the SiNW has been intentionally enlarged to 3:1 to deliver a better view.

Under such characterization, the $|E|^2$–x curve looks very like the side contour of a house. The peak light intensity (abbreviated as Peak-Int.) is 3720. Along the propagation direction, the light intensity shows the successive rapid increasing (L_1), slow increasing (L_2), slow decreasing (L_3), and rapid decreasing (L_4) variation trend. We chose the average value of the first wave crest and trough, 2701, as the criterion to separate the high and low light intensity. This criterion is called as the transom intensity (abbreviated as Tran-Int.). Such then, the lengths of L_1–L_4 are 0.07 μm, 1.21 μm, 0.98 μm, and 0.74 μm, respectively. And the distance mentioned above, which has the high level local light-harvesting amount (symbolized as L_{High}) can be determined as the summation of L_2 and L_3, 2.19 μm. Based on the light absorption formula $P_{abs} = I_{light} \cdot c \cdot \alpha$, the amount of light being absorbed P_{abs} is proportional to the light intensity I_{light}. Therefore, the Peak-Int. and Tran-Int. are naturally two criteria in measuring the LHE of the SiNW. However, L_{High} is not a good criterion as it is a quantity depends on the SiNW length. So, we define a relative quantity, the ratio between L_{High} and the whole length of the SiNW, L_{High}/L_{SiNW}, as the third criterion.

Then, we determine the optimal SiNW length for photovoltaic devices by comparing the LHE of SiNWs with various lengths 2–6 μm. As shown in the supplementary material,[21] the light intensity variations in the SiNWs with lengths 2, 4, and 6 μm show the similar trend as that in the SiNW with 3 μm length. In Fig. 4(a), we plot the Peak-Int. and the Tran-Int. of the SiNW with various lengths. It is easy to see that the Peak-Int. and the Tran-Int. in the SiNW with 3 μm length show the greatest values, which indicates that the light-harvesting amount in the L_{High} of SiNW with 3 μm length is greater than those with other lengths. The L_{High} for SiNWs with lengths 2, 4, and 6 μm are 1.44, 2.74, and 4.10 μm, respectively. And the corresponding L_{High}/L_{SiNW} (including that of the SiNW with 3 μm length) values are plotted in Fig. 4(b). The ratio of L_{High}/L_{SiNW} for the SiNW with 3 μm length is also the greatest, which is quite greater than those of the SiNW with 4 and 6 μm length, and slightly greater than that of the SiNW with 2 μm length. Comprehensively, the SiNW with 3 μm length not only has the greatest L_{High}/L_{SiNW} but also has the strongest light-harvesting ability in L_{High}, in the SiNWs with various lengths. This means that 3 μm should be the optimal SiNW length for photovoltaic applications.

The light intensity variation trend in Fig. 3 is quite different from that predicted from the Lambert-Beer law, based

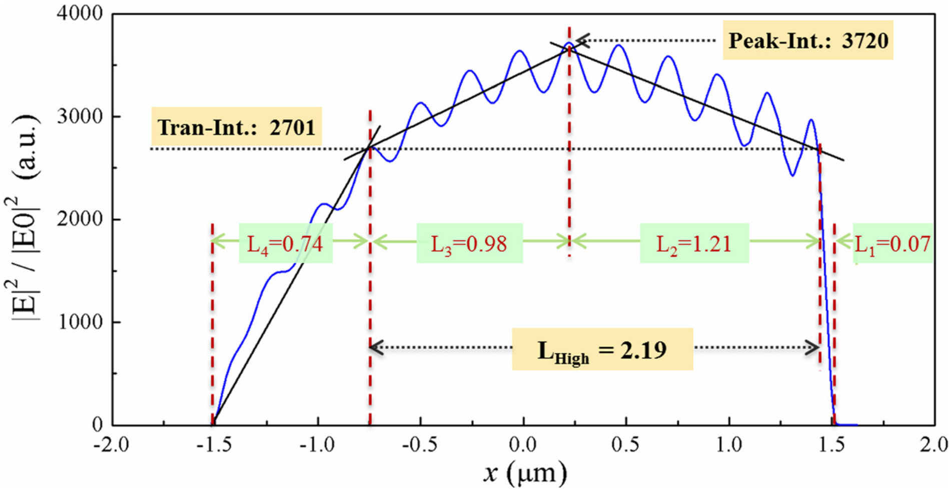

FIG. 3. The normalized variation curve of $|E|^2$ along the representative line within the SiNW.

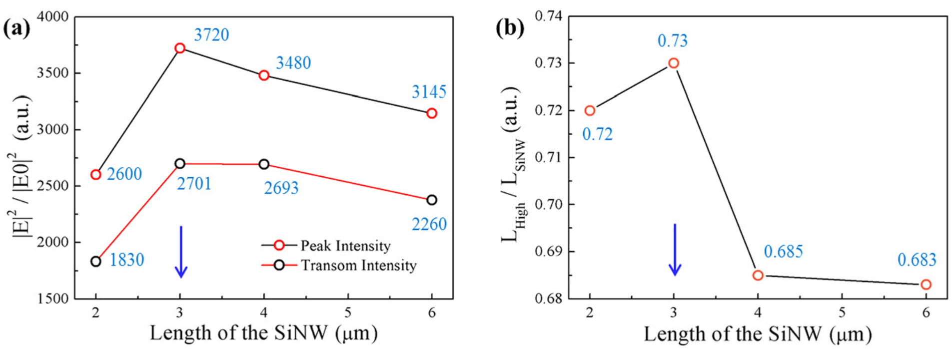

FIG. 4. (a) The peak and transom light intensities within the SiNW with various lengths. (b) The ratios between the length with high light intensity and the whole length of the SiNW, for SiNW with various lengths.

on which the light intensity will decrease monotonously. This phenomenon can be reasonably explained by the leaky mode excitation.[22,23] In segment L_1, the light in-coupling function of the leaky mode plays the leading role. Arriving at segment L_2, the leaky mode still plays the light in-coupling function but its working efficiency decrease since the light surround the SiNW becomes thinner than the incident light. Till segment L_3, the light absorption of the SiNW changes to be the dominant physical process, but the leaky mode still plays a light in-coupling function. This is because the decreasing rate of the light intensity is quite lower than that deduced from the Lambert-Beer law

$$I = I_0 \exp(-\alpha x), \tag{1}$$

where I_0 represents the light intensity at a start point, I is the light intensity when the light propagates a distance x, and α is the optical absorption coefficient of silicon which can be calculated by

$$\alpha(\omega) = \sqrt{2}\omega\left[\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} - \varepsilon_1(\omega)\right]^{1/2}, \tag{2}$$

where ω is the angular frequency of the light, ε_1 and ε_2, which equals to 17.695 and 0.3306 when $\lambda = 524$ nm, are the real and image part of the dielectric constant of silicon, respectively.

Taking the Peak-Int. in Fig. 3 as the start point, the light intensity should attenuate to be 1467 at the end of the segment L3 according to the Lambert-Beer law above. But actually, the light intensity is about 2701. In the last segment L_4, the leaky mode inversely plays a light leaking function since the actual light intensity at the end of the SiNW, 1, is significantly lower than that deduced from the Lambert-Beer law, 1338.

In conclusion, based on the investigations of the light intensity variations along the SiNW, we develop a method to determine the optimal SiNW length for photovoltaic devices. We find that the light exhibits a strange propagation feature along the SiNW. Its intensity shows a first increasing and then decreasing variation trend, and thus maintains high values over quite a long distance. Based on this feature, we propose three criteria to measure the LHE of the SiNW. By comparing the proposed criteria of SiNWs with various lengths, we conclude that the SiNW with length around 3 μm has the best LHE thus should be the optimal choice for photovoltaic applications. This value locates at the length range, in SiNW with which the enhanced light-harvesting can dominate over carrier recombination. We also give a reasonable explanation for the strange light propagation feature along the SiNW from the aspect of leaky mode excitation. This information is helpful in further exploiting the applications of SiNW in photovoltaics.

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