Optics Communications 355 (2015) 6–9

Contents lists available at ScienceDirect

Optics Communications

journal homepage: www.elsevier.com/locate/optcom

Linear length-dependent light-harvesting ability of silicon nanowire

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ARTICLE INFO

Article history:
Received 1 April 2015
Received in revised form
27 May 2015
Accepted 11 June 2015
Available online 15 June 2015

Keywords:
Silicon nanowire
Light-harvesting
Photovoltaic
Linear length-dependent

ABSTRACT

Silicon nanowire (SiNW) is of great promising for photovoltaic applications due to its excellent performance in light-harvesting. Some experimental and theoretical results indicate its light-harvesting is dramatically length dependent, while there is still no investigation on this dependency. Through reliable simulations on the optical extinction and absorption spectra of SiNWs with varying lengths, we find that the light-harvesting ability of SiNW is linear with its length. For the SiNWs of the optimal diameter, 80 nm, the linearity between the light-concentration (light-absorption) multiples and length is about 133 μm^{-1} (50 μm^{-1}). This linear relationship can be explained reasonably by the leaky modes theory.

1. Introduction

Silicon nanowire (SiNW) is of great promising for photovoltaic applications [1–5] due to that it can act as nanoantenna thus has excellent light-harvesting ability [6–10]. Several experimental reports [11–13] show that, the anti-reflective ability of SiNWs is dramatically length dependent. This phenomenon is consistent with the theoretical predictions [14]. In 1966, Lind et al. have calculated the the extinction spectrum of an infinite, model nanowire with index of refraction $m = 1.6$. Under illumination parallel to the nanowire axis, the obtained peak extinction efficiency (at “radius to wavelength ratio” about 0.7) is about 3.0. It should be noted that this value is calculated through dividing the extinction cross section by the normally projected geometric area of the nanowire, $2aL$, but not the cross sectional area, πa^2, for a nanowire of length L and radius a. By the latter strategy, the obtained extinction efficiency should turn to be infinite. This denotes that the light-harvesting ability of nanowire, including SiNW, should be infinite with its length.

Recently, following the flourish of photovoltaic devices based on SiNWs [5], many theoretical simulations on the optical properties of SiNW have been carried out [15–19]. But to the best of our knowledge, none of these studies focused on investigating the dependency of the SiNW's light-harvesting ability on length, which is helpful for the design of SiNW based solar cells. Therefore, further investigation on this issue is necessary.

Discrete dipole approximation (DDA) method [20–22] is very suitable in calculating the optical scattering and absorption of targets with arbitrary geometries, whose accuracy and reliability has been widely verified [23,24]. In this work, we investigate the length-dependence of the optical extinction and absorption efficiency of the SiNW. Our results reflect that the light-concentration and light-absorption abilities of the SiNW increase linearly with its length. These findings are of great help for the using of SiNW as blocks (e.g., as the light collector) in photovoltaic devices.

2. Model and simulation method

The SiNWs are modeled as circular cylinder with hemisphere tip, as shown in Fig. 1(a), to represent the real shape in experiments [9,25]. As the light-harvesting ability of SiNW array is not insensitive to the interspace between the nanowires [26], we only study the optical properties of single SiNW. Their diameters are all set as 80 nm, which is the optimized size for light-trapping [27]. (The fact that 80 nm is the best choice has been verified by us, through calculating the extinction efficiency spectra of nanowires with fixed length 1 μm and various diameters from 30 nm to 150 nm. Corresponding results are given in the supplementary materials.) Their lengths (barring the tip) vary from 0.027 μm to 13 μm, which is limited by the maximum processing power of the code we used. Besides, only the incident light from the top is considered, since the optical performance of SiNW is insensitive to

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http://dx.doi.org/10.1016/j.optcom.2015.06.027
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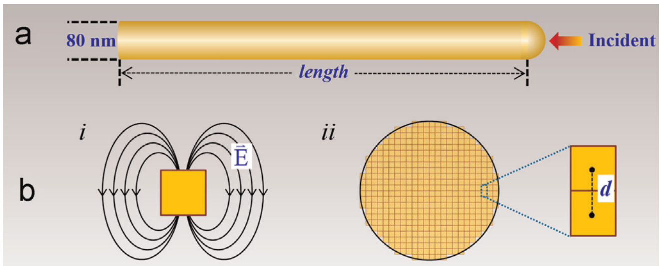

Fig. 1. (a) Schematic diagram of the SiNW. (b) Schematic diagram of (i) the square dipole used in DDA simulations, and (ii) the cross section of the SiNW composed of interacting dipoles with separation *d*.

the incident angle [28]. To help understanding, we provide a framework of the DDA method here.

The SiNW is replaced by a 3D collection of interacting point dipoles, located on cubic lattices, as shown in Fig. 1(b). These dipoles are indexed by $j=1,\ldots N$. The key problem is to determine a self-consistent set of dipole moments $\vec{P}_j$ by solving the set of 3 N linear equations

$$\sum_{k=1}^{N} A_{jk}\vec{P}_j = \vec{E}_{inc,j} \quad (j = 1, \ldots, N) \tag{1}$$

where $\vec{E}_{inc,j}$ is the electric field at position j due to the incident light, A_{jk} is the cross-interaction coefficient, and k is an index traversing all the dipoles. If two $3N$-dimensional vectors $\tilde{P} = (\vec{P}_1, \vec{P}_2, \ldots \vec{P}_N)$, $\tilde{E}_{inc} = (\vec{E}_{inc,1}, \vec{E}_{inc,2}, \ldots \vec{E}_{inc,N})$, and a $3N \times 3N$ matrix $\tilde{A}$ are defined, the problem can be reduced to a single matrix equation:

$$\tilde{A}\tilde{P} = \tilde{E} \tag{2}$$

This equation is solved by iterative methods, and the error tolerance between two adjacent iterative steps is specified as follows:

$$h = \frac{|\tilde{A}^{\dagger}\tilde{A}\tilde{P} - \tilde{A}^{\dagger}\tilde{E}|}{|\tilde{A}^{\dagger}\tilde{E}|} \tag{3}$$

where $\tilde{A}^{\dagger}$ is the hermitian conjugate of $\tilde{A}$. After the polarizations $\vec{P}_j$ are obtained, the extinction and absorption cross section are then computed as follows:

$$C_{ext} = \frac{4\pi\kappa}{|\vec{E}_0|^2}\sum_{j=1}^{N} \mathrm{Im}(\vec{E}_{inc,j}^{*}\cdot\vec{P}_j) \tag{4}$$

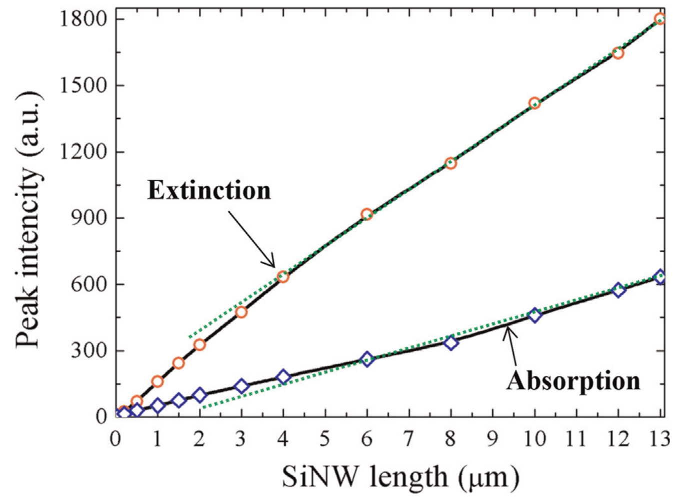

Fig. 3. Peak intensities in the extinction and absorption curves of SiNWs with varying lengths. The green dotted lines are plotted to guide eyes.

$$C_{abs} = \frac{4\pi\kappa}{|\vec{E}_0|^2}\sum_{j=1}^{N}\{\mathrm{Im}[\vec{P}_j\cdot(\alpha_j^{-1})^{*}\vec{P}_j^{*}] - \frac{2}{3}\kappa^3\vec{P}_j\cdot\vec{P}_j^{*}\} \tag{5}$$

where $\vec{E}_{inc,j}^{*}$ and $\vec{P}_j^{*}$ are the conjugate of $\vec{E}_{inc,j}$ and $\vec{P}_j$, respectively; $\kappa = 2\pi/\lambda$ (λ is the wavelength); $\vec{E}_0 = 1$ is the incident electric field intensity; α is the complex polarizability related to the dielectric constant of silicon. Then the corresponding extinction and absorption efficiency are written as follows:

$$Q_{ext} = C_{ext}/\pi r^2 \tag{6}$$

$$Q_{abs} = C_{abs}/\pi r^2 \tag{7}$$

where r is the real geometric radius of the SiNW. Such defined extinction and absorption efficiencies reflect the light-concentration and light-absorption ability, respectively.

The calculating accuracy of the DDA method mainly depends on two factors, the interdipole spacing d labeled in Fig. 1(b), and the error tolerance defined in Eq. (3). In our calculations, the values of d and h are both carefully tested, and set as 3.3 nm and 1.0×10^{-5}, respectively. The reliability of the DDA method has been ensured in our previous work [24].

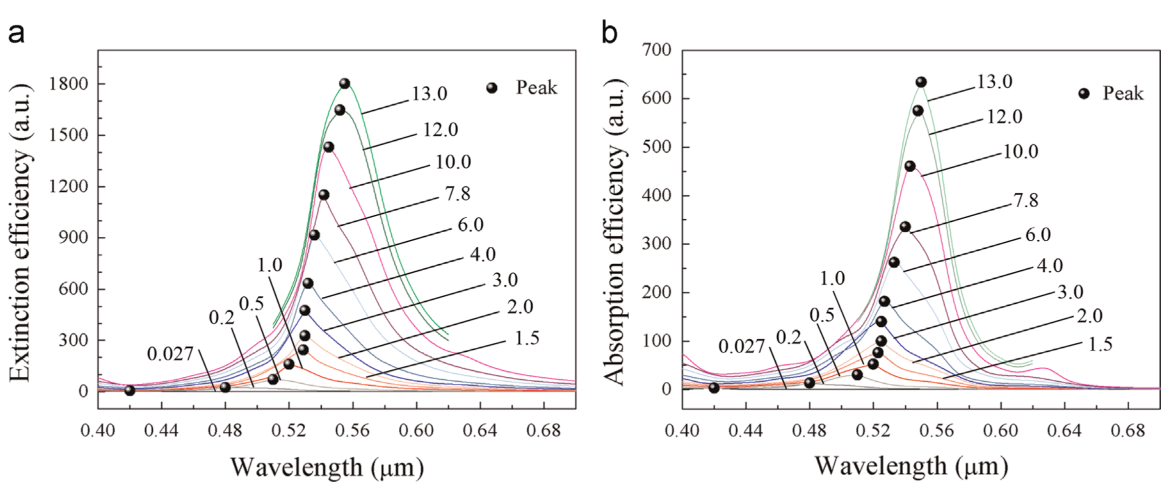

Fig. 2. Optical spectra of SiNWs with varying lengths from 0.027 μm to 13.0 μm. (a) Extinction efficiency curves. (b) Absorption efficiency curves.

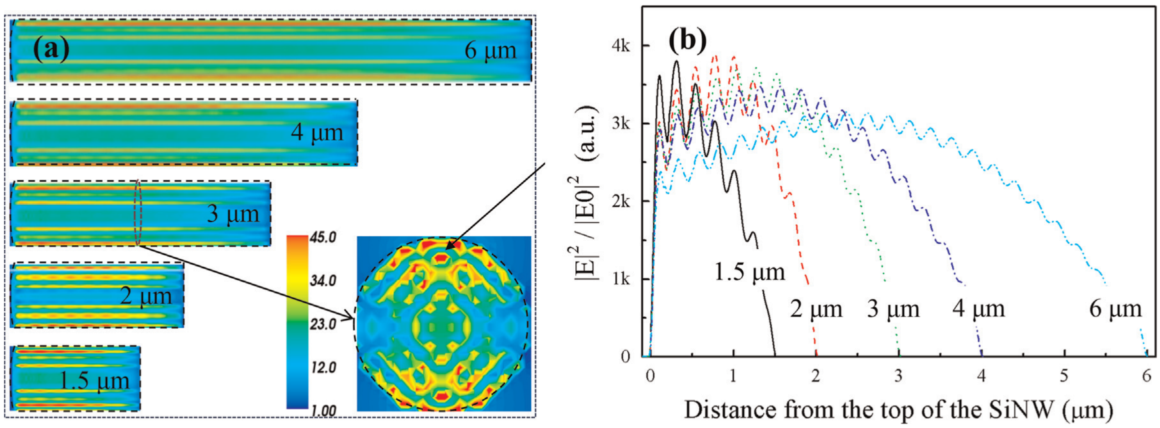

Fig. 4. (a) Electric field (|*E*|) distributions in the vertical sections of SiNWs with varying lengths and index for the position where the |*E*| used in (b) are extracted from. (b) Variation trend of the light intensity ($|E|^2/|E_0|^2$, $E_0=1$ denotes the incident electric field) from the top of the SiNWs with varying lengths.

3. Results and discussions

To investigate the length-dependence of the light-harvesting ability of SiNW, as a start, we carry out simulations on the the extinction and absorption efficiency curves of the SiNWs with varying lengths, as shown in Fig. 2(a) and (b). Both of them show dramatic dependence on the SiNW's length: they increase with the length. Such a law is the most obvious at the resonance wavelengths of the SiNWs, as marked by black spheres in Fig. 2. From the variation trends of these marked spheres, two key messages can be found. The first one is that the resonance wavelengths of the SiNWs will approach a fixed value with the length increase, which indicates the resonance wavelength should be mainly diameter-dependent. The second one is the light-concentration and light-absorption abilities of the SiNW both increase continuously with the length. This continuous increasing trend means that an infinite SiNW should own infinite light-harvesting ability, which is consistent with the conclusion derived from Lind et al.'s [14] work.

Then, with the aim to find out the length-dependency of the SiNW's light-harvesting ability, we pick out the peak intensities in the extinction and absorption curves and plot them as a function of the SiNW length in Fig. 3. On a brighter note, both the extinction and absorption efficiencies exhibit linear relationships with length, and the linearity is nearly perfect when the length are greater than 4 µm. As guided by the green dotted lines, the slopes of these two lines are about 133 μm^{-1} and 50 μm^{-1}, respectively. The imperfect linearity, when the lengths are smaller than 4 µm, can be ascribed to the hemisphere tip on the SiNW.

The physical image behind above linear relationship can be intuitively reflected by the electric field distributions within the SiNWs, as shown in Fig. 4(a). This is because the square of electric field intensity represents the local light intensity within the SiNW. For more clearly, we choice a representative lines in every SiNW (whose projection in cross section has the maximum electric field intensity), extract the |*E*| values along these lines and take them squared, and plot $|E|^2/|E_0|^2$ as a function of the distances from the top of the SiNWs in Fig. 4(b). It can be seen that, for each SiNW, there is a long range owning great light intensity. Such light intensities are nearly the same in SiNWs with different lengths. And the length of the range (owning great and approximate light intensity) depends dramatically on the whole length of the SiNW.

The reason for this linear increasing light-harvesting ability with lengths can be reasonably attributed to the leaky modes excitation [29] in SiNW. The leaky modes has an electromagnetic field that decays monotonically for a finite distance in the transverse direction (i.e., at a 90° angle to the axis of the SiNW), but becomes oscillatory beyond that finite distance [30]. This oscillatory electromagnetic field can act like an antenna and thus couple the surroundings light field into the SiNW. The oscillatory feature of the leaky mode signifies that the SiNW can affect an infinite range thus can couple more and more light into it with its length increase.

Based on the above researches, we find that the light-harvesting ability of SiNW is linear with length. Such linear relationships imply that, from the perspective of pure optical absorption, the length of the SiNW used in fabricating photovoltaic devices should be the long the better. However, the performance of SiNW based photovoltaic devices depends not only on the SiNW's light-absorption ability but also on the carrier transport length. The light-absorption ability determines the amount of carriers generated, while, the carrier transport distance determines how many of the generated carriers can be exported thus converted to photocurrent. Under such considerations, the optimal length of SiNW used in actual photovoltaic devices should be independent on its optical performance but determined by its electric properties.

4. Conclusion

In conclusion, based on studies on the light-concentration and light-absorption abilities of SiNWs with varying lengths from 0.027 µm to 13 µm, we find that the light-harvesting ability of SiNW increases linearly with its length. In the specific case where the diameter of the SiNWs is 80 nm, the linearity between the light-concentration multiples and the length is about 133 μm^{-1}, and that of the light-absorption multiples is 50 μm^{-1}. Such linear relationships can be reasonably explained by the leaky modes excitation in the SiNW. These findings mean that, in designing SiNW based photovoltaic devices, its length is the long the better from optical perspective.

Acknowledgments

This work was supported partially by the National Natural Science Foundation of China (Grant nos. 91333122, 51402106, 51372082, 51172069, 50972032, 61204064 and 51202067), Ph.D. Programs Foundation of Ministry of Education of China (Grant nos. 20110036110006, 20120036120006, 20130036110012), Par-Eu Scholars Program and the Fundamental Research Funds for the Central Universities.

Appendix A. Supplementary material

Supplementary data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.optcom.2015.06.027.

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