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Linear length-dependent light-harvesting ability of silicon nanowire

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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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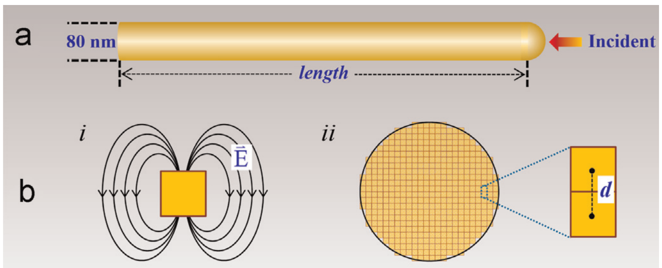

Fig. 1. (a) Schematic diagram of the SiNW. (b) Schematic diagram of (i) the square dipole used in DDA simulations, and (ii) the cross section of the SiNW composed of interacting dipoles with separation *d*.

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:

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

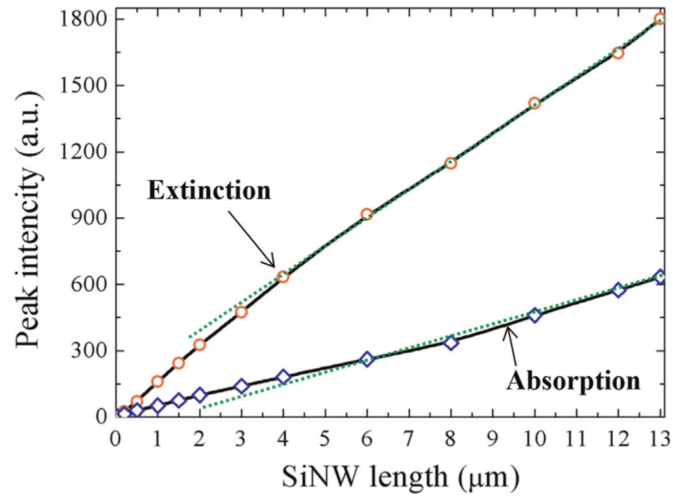

Fig. 3. Peak intensities in the extinction and absorption curves of SiNWs with varying lengths. The green dotted lines are plotted to guide eyes.

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

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].

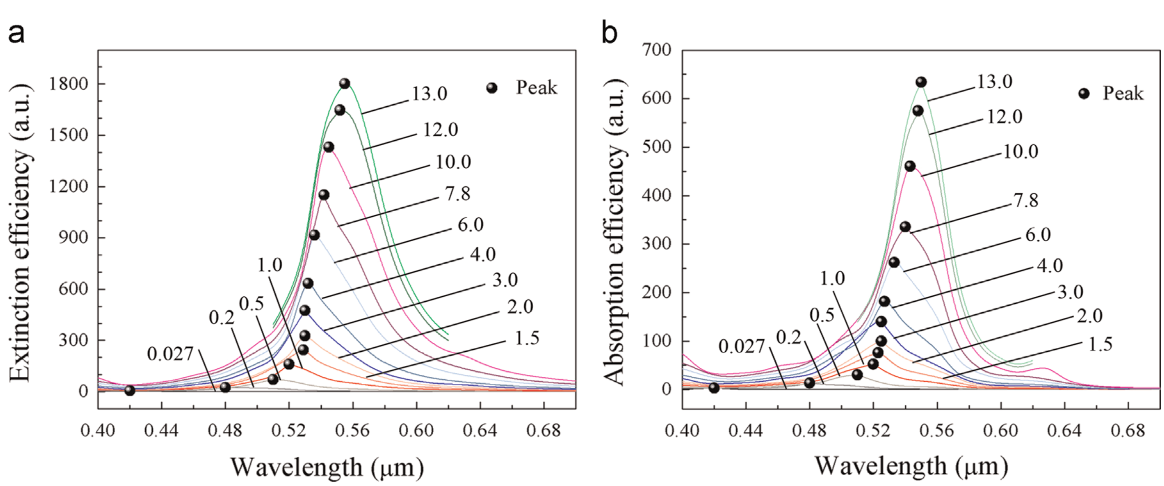

Fig. 2. Optical spectra of SiNWs with varying lengths from 0.027 μm to 13.0 μm. (a) Extinction efficiency curves. (b) Absorption efficiency curves.