

Optical absorption enhancement in disordered vertical silicon nanowire arrays for photovoltaic applications

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Optical properties are numerically investigated for vertically aligned silicon nanowire arrays with three types of structural randomness, i.e., random position, diameter, and length. Nanowire arrays with random position show slight absorption enhancement, while those with random diameter or length show significant absorption enhancement, which is attributed to the stronger optical scattering in a random structure. Our results indicate that structural randomness in vertical nanowire arrays will not destroy but rather can further enhance optical absorption compared to ordered nanowire arrays. © 2010 Optical Society of America

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Silicon nanowire (NW) arrays have received considerable attention recently for solar cell applications [1–3]. The radial p - n junction can enable efficient carrier collection [4], and the open array structure can significantly enhance optical absorption [2,5]. Absorption enhancement can be attributed to three major mechanisms. First, the NW array structure has remarkably small reflectivity owing to the large open area on the frontal surface. Second, each individual NW is a nanoscale cylindrical resonator, which can trap light by multiple total internal reflections [6]. Third, strong interwire light scattering occurs to cause further light trapping [7,8] because the NW diameter and period are normally of the same order as the optical wavelength. These mechanisms are quite sensitive to structural parameters of the NW array. So far, most experimental and all theoretical works have concerned ordered arrays with uniform NW diameter and length [9,10]. However, various types of structural randomness, such as random NW position, diameter, length, and orientation, are inevitable in experimentally synthesized devices. In fact, a few experiments have been performed on NW arrays with random orientation (and probably random length, diameter, and position as well) [7,11], and increased reflection or backscattering is generally observed but the effects on absorption are not clear. On the other hand, our previous studies on a random one-dimensional multilayer and two-dimensional cylinders have indicated significant absorption enhancement due to photon localization in random media [12–14]. Therefore, it is necessary to evaluate whether each type of structural randomness will deteriorate the excellent absorption of NW arrays or, on the other hand, has the potential to further enhance absorption.

In this Letter, we numerically investigate the impacts of three types of structural randomness on light absorption, including random position, diameter, and length. The reflection, transmission, and absorption of these NW arrays are predicted and compared with those of ordered arrays.

We will first discuss random position and diameter. The xy plane of the simulation domain is a 800 by

800 nm square with periodic boundary conditions, and the z dimension is truncated by the perfectly matched layers. The xy plane is divided into 16 200 by 200 nm cells, and 16 vertical NWs without substrate are used. For random NW position, one NW of 100 nm diameter is placed randomly within each cell. For random NW diameter, the diameter is randomly chosen from 60 to 140 nm and the center of each NW is located at the center of each cell. The NW length is fixed at 2 μm . The structures are shown in Fig. 1. The MIT Electromagnetic Equation Propagation package [15], based on the finite-difference time-domain (FDTD) method, is employed. The silicon dielectric function is adopted from the literature [16]. A spatial resolution $\Delta x = 10$ nm is chosen and the time step Δt is given by $0.5\Delta x/c$, where c is the speed of light. A source plane, which generates linear-polarized planar waves, is located 1 μm above the NWs. The incident photon frequency is studied in the range of 1.6 to 3.0 eV with a 0.05 eV interval. The reflectance, transmittance, and absorptance at each frequency are calculated using the respective energy flows, as used in our prior work on carbon-nanotube arrays [8]. For each type of

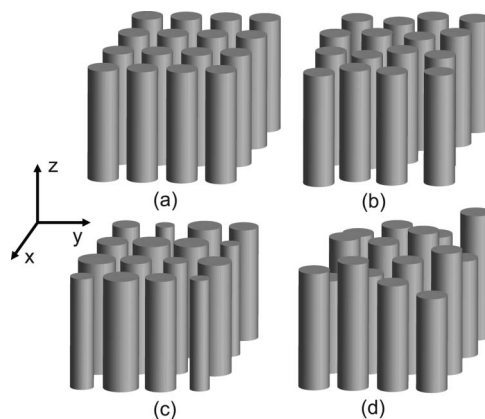


Fig. 1. Sketches of ordered and random arrays: (a) ordered, (b) random-position, (c) random-diameter, and (d) random-length.

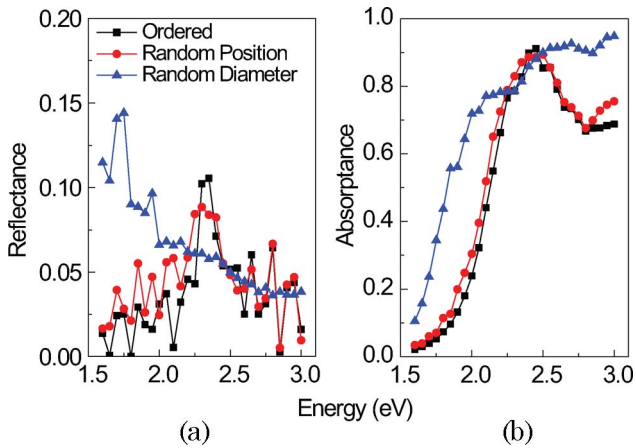


Fig. 2. (Color online) (a) Reflectance and (b) absorbance of ordered and random silicon NW arrays from FDTD calculations.

randomness, eight distinct configurations are sampled and the results are averaged.

The calculated reflectance data of the ordered and random arrays are shown in Fig. 2(a). The frequency-dependent reflectance of the ordered array is characterized by some oscillations and an evident peak at 2.35 eV. The random-position array shows a similar reflectance profile while the peak slightly shifts to lower frequency. The random-diameter array, in contrast, shows slightly higher reflectance at low frequency and nonoscillating reflectance at higher frequency. The results indicate that frequency dependence is primarily determined by the NW diameters, while their positions only slightly affect the reflectance profile. Also, the reflectances of random position and diameter NW arrays are still quite low and comparable to the ordered array, because forward scattering dominates over backscattering when light strikes on the vertical NW arrays. They differ from those arrays with completely random orientations, where the scattering is nearly isotropic [7], and the reflectance can be as large as 60% [11].

As shown in Fig. 2(b), the absorbance of the ordered array shows a general increase with frequency owing to the increase of the absorption coefficient of silicon. An absorption peak is located at 2.4 eV, which is consistent with the experimental absorption peak of an individual silicon NW with the same diameter reported in [6]. This peak was attributed to the internal resonance [6]. These resonance modes can further induce field enhancement and absorption peaks at certain frequencies. Because of the large aspect ratio of NWs, the resonance frequencies are determined by the diameters but not length. Figure 3(a) shows the energy density on a vertical cross section of a NW under the illumination of two different frequencies. Clearly, the 2.4 eV source induces larger field enhancement than the 2.7 eV one. This explains why the NW array has stronger absorption at 2.4 eV than 2.7 eV, even though silicon is more absorptive at the latter frequency. For the random-position NW array, the absorption peak is preserved, because the diameter remains uniform. The overall absorbance is slightly larger than ordered NWs, indicating enhanced multiple scattering and extended optical path length. In the case of a random-diameter array, there is no evident absorption peak, because different diameters give different resonance fre-

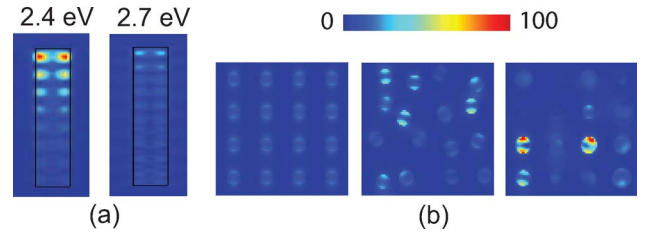


Fig. 3. (Color online) (a) Energy densities of an individual NW at two different frequencies. (b) Energy density distributions at an xy cross section of ordered, random-position, and random-diameter NW array. Single-frequency continuous sources are used to generate the plots. The color bar shows the ratio of the energy density to the incident energy density.

quencies as well as absorption peaks. As such, the absorbance is significantly broadened and enhanced for those originally off-resonance frequencies. Interestingly, the absorbance at the original resonance frequency is not deteriorated, although most NWs are no longer at this diameter. This indicates significant enhancement of multiple scattering induced by the random arrangement or diameter, similar to those observed in two-dimensional random media [12]. Although the randomness here is not along the incident direction, the incident wave is diffracted by this subwavelength structure and then multiply scattered. To show the internal resonance and scattering effects more clearly, the energy densities at a horizontal cross section of the three different NW arrays are plotted in Fig. 3(b). In the ordered array, each individual NW has a resonance mode characterized by two lobes (the source is polarized in the y direction). NWs in the random-position array have a similar mode profile, but the electric and magnetic fields are further enhanced because of the enhanced scattering within random media. In the random-diameter array, different NWs have different mode profiles and even stronger field enhancement is seen.

Random lengths can be introduced on purpose to further suppress the reflection. Numerical calculations have shown that less-dense NW arrays have smaller reflection [5]. However, sufficient volume fraction is still needed to effectively absorb light. To overcome this dilemma, modifications of the structures have been proposed, such as the dual-diameter arrays [17] and nanocone array [18], which create either an intermediate layer with small local volume fraction or a gradually varying volume fraction. Therefore, the dielectric contrast as well as reflection are reduced. Alternatively, we propose to use an NW array with random lengths, which can also generate varying volume fraction, hence reducing reflection. In addition, random length is expected to induce multiple scattering and field localization, analogous to the random textured surface in thin-film solar cells [19]. Such a structure is much simpler than the nanocone and dual-diameter structures.

To investigate the effects of random length, we use NWs with ordered position and uniform diameter. Two different sets of diameter are simulated, including 100 and 160 nm, and the corresponding arrays have a volume fraction f of 0.2 and 0.5, respectively. The lengths are randomly picked from 1 to $2\ \mu\text{m}$ with a uniform probability distribution. The average length is thus $1.5\ \mu\text{m}$.

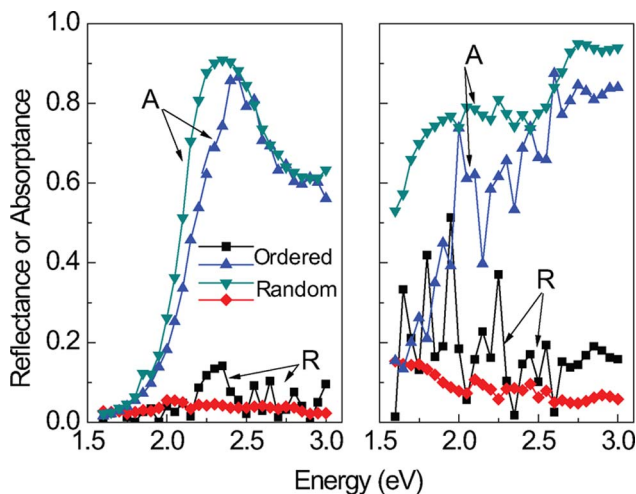


Fig. 4. (Color online) Reflectance and absorbance of ordered and random-length NW array with volume fraction of 0.2 (left) and 0.5 (right). *R* denotes reflectance and *A* denotes absorbance.

The lower surfaces of all NWs are kept on the same plane; hence, a rough top surface with a roughness of $1\ \mu\text{m}$ is created. The calculated reflectance and absorbance are compared with those of uniform length ($1.5\ \mu\text{m}$), as shown in Fig. 4. The absorption is significantly enhanced for both volume fractions, and the reflectance does not oscillate with the frequency any more owing to the rough top surface. For the $f = 0.2$ case, the reduction of reflectance is not significant, since it is already quite small, so the enhanced absorption is mostly due to the optical scattering induced by the random top surface. In contrast, the suppression of reflectance is significant for the $f = 0.5$ case.

In summary, numerical calculations are carried out to investigate the NW arrays with random position, diameter, and length. Compared to an ordered NW array, the random-position NW arrays have a similar reflection profile but slightly enhanced absorption. Random-diameter arrays show significantly broadened and enhanced absorption, and random-length NW arrays show both significantly reduced reflection and enhanced absorption. The absorption enhancement can be attributed to the enhanced interwire multiple scattering and/or inner-wire resonance in the random array structure. Our results indicate that randomness in position, diameter, and length is beneficial for optical absorption. Therefore, it is unnecessary to take extra steps in experi-

mental synthesis to eliminate these types of randomness, but rather, they should be purposely introduced, designed, and optimized beyond the level of just natural randomness.

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