Broadband absorption enhancement in randomly positioned silicon nanowire arrays for solar cell applications

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In this Letter, the optical properties of randomly positioned silicon nanowire arrays are studied. The result shows that position randomization with a filling ratio larger than 36% renders better absorptance over a broadband ranging from 300 to 1130 nm compared to regular structures. The ultimate efficiency of a 48% filling ratio position randomized nanowire structure is 13.4% higher compared to the optimized regularly arranged nanowire structure with the same thickness. The absorptance enhancement of random structures is attributed to lowered reflectance, more supported resonant modes, and broadening of existing resonance.

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Silicon solar cell is presently dominating the solar cell market owing to the abundant supply, nearly ideal bandgap, and mature fabrication process. Most commercial silicon solar cells are wafer-based cells with thickness of a few hundred micrometers, which consume a large amount of silicon, leading to a high cost of the final product [1]. However, the weak absorption, especially in the long wavelength range near the bandgap edge of silicon, remains a problem. Silicon nanowire (NW) structures are promising to achieve thin yet efficient solar cells and have been studied intensively owing to the large enhancement of absorption and improvement of carrier collection [2–13]. Besides, other nanostructures, such as nanohole [14,15], nanocone [16], and nano-cone-hole [17] have also been proposed for photovoltaic applications. Thus far, most of the experimental and theoretical work is focused on regularly arranged nanostructure arrays with square or triangular lattice. Optimal lattice constant and silicon filling ratio of NW arrays have been obtained to achieve a high ultimate efficiency [9,10]. On the other hand, randomly positioned NW arrays are of much lower cost as it is difficult and costly to maintain the large area regularity with a few hundreds of nanometers' registration. A few experimental works on NW arrays with random orientation, length, size, and position show increased reflection [8,18]. Theoretically, it has been reported that structural disorder can introduce additional resonances and broaden existing resonances [19]. Recently, it has been reported by Bao and Ruan that optical absorption could be enhanced with disordered vertical silicon NW arrays in the wavelength range from 410 to 775 nm [20]. The random structure considered in [20] is generated by randomly placing the NW within its unit cell while keeping the unit cell position fixed, which is a special case of position random structures. The influence of a general case position randomization on the optical properties has not been studied yet. In this Letter, we investigate the optical properties, including absorptance, reflectance, and transmittance of general case position randomized NW structures.

Figure 1 shows the schematics of the NW arrays for the study. All considered structures are arranged in an x–y plane and surrounded by air. Sunlight is directly incident on the top of the structure along z direction. The regularly arranged NW array in a square lattice is shown in Fig. 1(a).

According to the optimal parameters [9], the lattice constant (period) is chosen as 500 nm, and the filling ratio (defined as the ratio of the NW top surface area to the unit cell top surface area in one unit cell) is 0.5, which means the radius of the NW is about 199 nm, which is used for all structures in this paper for easy comparison. Periodic boundary conditions are used in x, y directions and a perfectly matched layer boundary condition is used

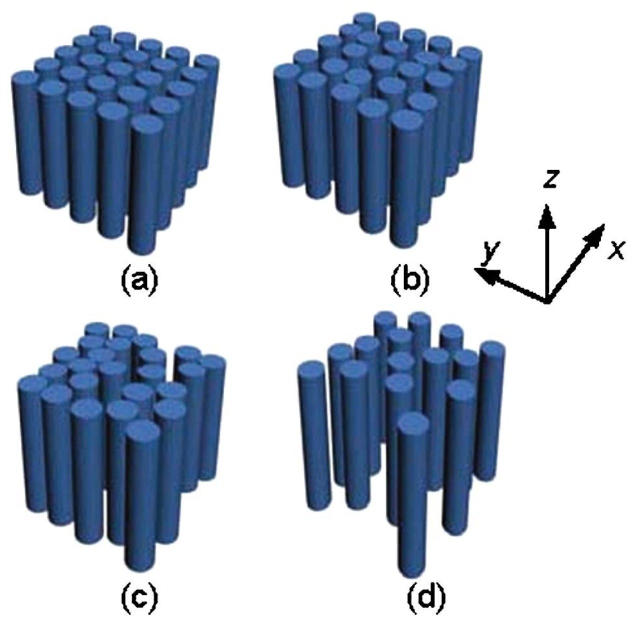

Fig. 1. (Color online) Schematics of silicon NW arrays with a (a) regularly arranged square lattice, (b) random NW contained in regular unit cell used in [20], (c) 48% position random, and (d) 30% position random structure.

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in z direction. Five periods are chosen in x and y directions leading to a simulation region of a $2.5\,\mu$m by $2.5\,\mu$m square area in the x–y plane. The same boundary condition and simulation region are used for all random NW structures. Figure 1(b) shows the position random structure as [20] with the NW randomly placed within the unit cell containing it (i.e., the largest displacement of any NW is 40 nm from its original position in the regular structure), which is called random NW contained in regular unit cell NW array. Figure 1(c) shows a general case position randomized NW array. For the general case position random NW array, the filling ratio is generally lower than the regularly arranged NW array. In our case here, the filling ratio is 48%; the structure is called 48% position random NW array. A general case position randomized NW array with a 30% filling ratio is shown in Fig. 1(d) and named as 30% position random NW array for short. In the process of generating position random NW arrays, the NW overlapping cases were excluded. In our analysis, the thickness of all NW arrays is fixed at $2.33\,\mu$m similar to [4] and the finite-difference time-domain (FDTD) method is employed for all spectra calculation using Lumerical FDTD Solutions, a commercial FDTD software package. For all random NW structures in Figs. 1(b)–1(d), four different structures are simulated and then averaged to avoid any small probability event. The silicon dielectric function used is taken from [21].

Figure 2(a) shows the absorptance spectra of four different 48% position random NW arrays. The four NW structures are randomly generated by the computer. The corresponding random structures of the four cases are shown in the figure inset. From Fig. 2(a), the absorptance spectra of the four cases are close to each other with little deviation. Similar results were also obtained for position random NW arrays with other filling ratios we have tested. Thus, it is meaningful to use the average (or any one) of the absorptance spectra of the 48% position random NW arrays to compare with the standard regular structure and other filling ratio position random NW arrays.

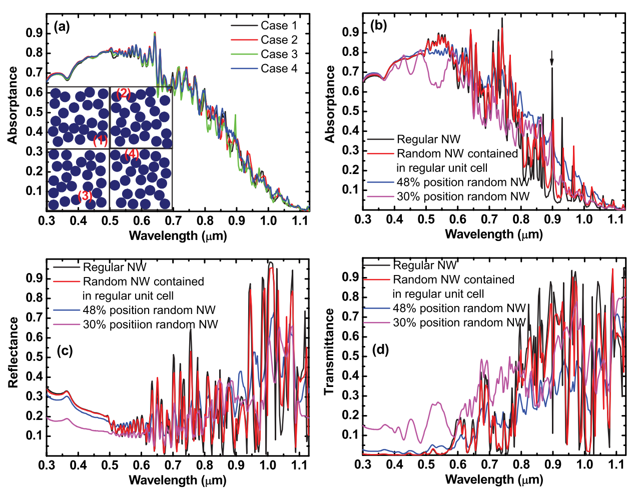

Fig. 2. (Color online) (a) Absorptance of four different 48% position random NW arrays. (b) Absorptance, (c) reflectance, and (d) transmittance of regular, random NW contained in regular unit cell, 48% position random, and 30% position random silicon NW arrays, respectively.

Figures 2(b)–2(d) show the optical properties of the four structures shown in Fig. 1. Each absorptance peak in the spectra corresponds to a guided resonant mode [9,15]. From Fig. 2(b), the absorptance of random NW contained in a regular unit cell NW array is close to that of the regularly arranged NW array in the wavelength range considered here, i.e., this random structure does not have much influence on the absorptance. Small deviations from the original position do not lead to an obvious increase in supporting modes and mode broadening, which is consistent with the analysis in [20]. The reflectance [Fig. 2(c)] and transmittance [Fig. 2(d)] of the regular array are also similar to those of regularly arranged one. As shown in Fig. 2(b), the absorptance of the 48% position random NW array is significantly higher and flatter compared to both the random NW contained in regular unit cell and regularly arranged NW arrays in long wavelength range from 800 nm to $1.13\,\mu$m where the absorption is very weak, a problem suffered by thin-film silicon solar cells. The corresponding reflectance and transmittance are also shown in Figs. 2(c) and 2(d). In the short wavelength range, the absorptance is mainly determined by the reflectance owing to the high material absorption of silicon in this range. The lower the reflectance, the higher the absorptance is. From Fig. 2(c), the reflectance is similar for all NW arrays, which results in a similar absorption in the short wavelength range. The transmittance [Fig. 2(d)] is close to zero in the short wavelength range. In the long wavelength range, the absorptance is determined by both reflectance and the supported guided resonant modes. From Fig. 2(c), the reflectance of the 48% position random NW array is lower than the random NW contained in regular unit cell and the regularly arranged NW arrays, which are confirmed by the transmittance in Fig. 2(d). Besides, the structural disorder introduces additional resonances and broadens existing resonances leading to an absorption enhancement [19]. More modes are induced for larger position randomness. The flatter absorption spectrum of a position random NW array indicates that the resonances are more broadened. The optical properties of a NW array as a function of the filling ratio are further investigated for general case position random NW arrays. Even when the NW filling ratio is 30%, the absorptance is only slightly lower than that of the regularly arranged one. From Fig. 2(c), the 30% position random NW array has better antireflection performance. The reflectance is lower than that of the regularly arranged array. The drop of absorptance is mainly coming from the less supported resonant modes when the filling ratio becomes lower. With less supporting modes, light cannot be trapped in NW structures long enough to enhance absorption. Hence, a larger transmittance in all considered wavelength ranges is expected compared to others [Fig. 2(d)].

In Fig. 3, we plotted the electric- (E-) field intensity distributions in the regular structure and the 48% position random structure at two wavelengths of $\lambda = 899.1$ nm and $\lambda = 916.0$ nm. These two wavelengths were chosen as 899.1 nm is one absorptance peak and 916.0 nm is the next adjacent absorptance trough for the regularly arranged NW array [Fig. 2(b)]. It is clear by comparing Figs. 3(a) and 3(b) with Figs. 3(c) and 3(d) that the resonance corresponding to the 899.1 nm wavelength has

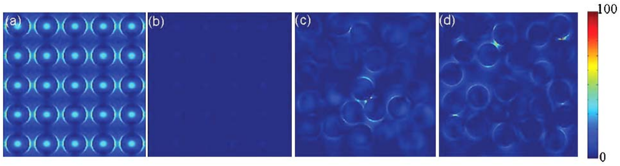

Fig. 3. (Color online) E-field distributions in a regularly arranged NW array at (a) $\lambda = 899.1$ nm and (b) $\lambda = 916.0$ nm. E-field distributions in a 48% position random NW array at (c) $\lambda = 899.1$ nm and (d) $\lambda = 916.0$ nm.

been broadened by introducing the randomization. Moreover, we can also see from Fig. 3(d) that an additional mode appears at 916.0 nm. The broadening of resonance can also be understood from the quality factor (Q factor). The sharp peaks in the absorptance spectrum of a regularly arranged structure correspond to guided resonant modes with high Q factor [Fig. 2(b)]. The higher the Q factor, the longer the light will be trapped in the structure attributing to a higher absorptance peak. With randomization introduced to the regular structure, the Q factor is reduced. The reduction of the Q factor leads to a broadening of the resonance, hence, broadening of the absorption spectrum.

The ultimate efficiencies [22] for all cases were calculated under Air Mass 1.5 (AM1.5) [23] irradiation and are shown in Table 1. The efficiency of regularly arranged, random NW contained in regular unit cell, 48% position random, and 30% position random NW arrays is 26.12%, 27.39%, 29.61%, and 24.53%, respectively. It additionally verifies that the absorptance of random NW contained in a regular unit cell NW array is only slightly better than the regularly arranged one. The ultimate efficiency of the 30% position random NW array is only slightly lower than that of the regularly arranged NW array. The ultimate efficiencies of other filling ratios were also calculated. Our results show that the ultimate efficiency is always larger than that of the regularly arranged one for position random structures with a filling ratio larger than 36%. The ultimate efficiency of the 48% position random NW array is 15% improved compared to the regularly arranged array. Thus, the efficiency of general case position random NW arrays has better performance compared to others.

In conclusion, optical properties of various random NW arrays are studied in detail. Better absorption performance of random structure is owing to better antireflective performance, additional resonances introduced by the structural disorder, and existing resonances broadening. With comparable filling ratio, more randomness leads to larger absorption enhancement. Our results here indicate that high performance silicon NW solar cells can be obtained by low-cost bottom-up approaches.

Table 1. Ultimate Efficiency of Various NW Arrays

NW Arrays	Regularly Arranged	48% Position Random	Random NW in a Regular Unit Cell	30% Position Random
Ultimate efficiency	26.12%	29.61%	27.39%	24.53%
Enhancement		13.4%	4.8%	–6.1%

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