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Geometric parameter optimization to minimize the light-reflection losses of regular vertical silicon nanorod arrays used for solar cells

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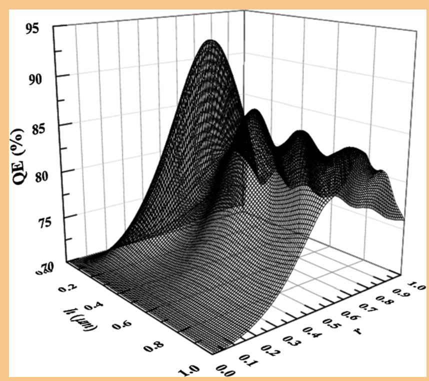
We theoretically investigate the light-reflection properties of silicon nanorod (SiNR) arrays with square and hexagonal alignments. The reflectivity of photon flux (RPF) is introduced to evaluate the light-reflection capability of SiNR arrays. The quantum efficiency (QE) varies on changing the geometric parameters of SiNR arrays. The optimal geometric parameters of SiNR arrays corresponding to maximum QE of 92.4% are achieved. The optimum ratio (SiNR diameter divided by the array periodicity) is 0.72 for the square arrays and 0.67 for the hexagonal arrays, and the optimum SiNR length for both alignments is the same with a value of 0.090 μm. In addition, the optimal geometric parameters are independent of the array density.



1 Introduction Studies of silicon nanowire (SiNW) arrays in solar cells have been the focus of researchers due to their advantages and good performances [1, 2]. Different novel photovoltaic devices based on SiNW arrays have been designed in succession [3, 4]. Meanwhile, the effect of the geometric parameters of SiNW arrays on the optical properties is receiving wide attention. Some studies have shown that the disordered nanostructures tend to have higher efficiencies than ordered structures [5–7]. However, other studies have revealed that the disorder in the location of nanowires does not affect the absorption spectrum [8] and the periodically aligned arrays have excellent antireflection properties with a low reflection loss for incident light [9]. Studies on ordered arrays have shown that the light reflectance of SiNW arrays is much lower than in a silicon film with the same thickness, and it is sensitive to the volume filling ratio, the SiNW diameter and length, the array periodicity, and the ratio of SiNW diameter to the array periodicity [10–15]. So far, there is still considerable debate regarding the effects of the above geometric parameters due to the difference in the samples used. Moreover, the results of theoretical simulation relate closely to the different approximation methods of gradient refractive-index coating [16, 17], and the optimal design can only be achieved with a careful choice of adjustable parameters. However, regarding the silicon nanorod (SiNR) arrays that are highly ordered, the effective refractive index can be approximated to be constant and there is no transition layer with the gradient refractive index, so the optimum geometric parameters can be obtained theoretically.

2 Theoretical model In this letter, based on the analyses of the reflectivity of photon flux (RPF) and the calculations of the quantum efficiency (QE), the optimal geometric parameters of SiNR arrays are obtained and discussed. RPF is defined as follows:

$$\mathrm{RPF} = \frac{F(\lambda)R(\lambda)\lambda}{h_0 c_0}, \tag{1}$$

where $F(\lambda)$ is the distribution of spectral intensity in $\mathrm{Wm^{-2}\,\mu m^{-1}}$ under AM 1.5 and given by Planck's radiation law. $R(\lambda)$ is the effective light reflectivity of SiNR arrays coating and calculated by the transfer matrix methods [18]. λ is the wavelength of incident light and it is set within the range of 0.310–1.127 μm. h_0 and c_0 are Planck's constant and the speed of light in vacuum, respectively. RPF represents the number distribution of reflected photons under the different wavelengths, and it is influenced by a variety of geometric parameters of SiNR arrays. $\mathrm{QE} = (\Phi_\mathrm{I}–\Phi_\mathrm{R})/\Phi_\mathrm{I}$, where Φ_I is the incident photon flux, Φ_R is the reflected photon flux. Here, it is assumed that the reflection is the only means of photons loss, and the left photons can be converted completely to electron–hole pairs that each absorbed photon with energy greater than the bandgap produces one and only one electron–hole pair.

Based on the above assumption, the light-reflection capability of SiNR arrays can be evaluated by comparing the number of reflected photons. The smaller the number of reflected photons, the lower the light-reflection capability of SiNR arrays, which results in higher QE and vice versa. So, the optimized optical geometric parameters of SiNR arrays can be obtained by reducing the number of reflected photons to the minimum for solar cells. For the square and hexagonal arrays, we analyze how the different geometric parameters affect QE and RPF, and finally find the optimal diameter and length of SiNR arrays.

In our calculations, the silicon substrate, of semi-infinite thickness, is covered with a single-layer homogeneous SiNR arrays coating at the air/silicon interface. The length of regular vertical SiNR arrays is h and the incident light is normal to the silicon substrate as shown in Fig. 1a. The effective refractive index n_EFF of an SiNR array coating can be calculated according to the effective medium approximation [18, 19] and it exhibits a step-like distribution,

$$\frac{f_1\left(n_\mathrm{Si}^2 - n_\mathrm{Eff}^2\right)}{\left(n_\mathrm{Si}^2 + 2n_\mathrm{Eff}^2\right)} + \frac{f_2\left(n_\mathrm{Air}^2 - n_\mathrm{Eff}^2\right)}{\left(n_\mathrm{Air}^2 + 2n_\mathrm{Eff}^2\right)} = 0, \tag{2}$$

where f_1, f_2 are the ratio of volume filling of SiNPs and the air, respectively, and $f_1 + f_2 = 1$. n_Si, n_Air, and n_Eff are the refractive indices of silicon, the air and the interlayer of SiNPs, respectively. As shown in the inset of Fig. 1b, L is the period length, D is the diameter of SiNR, and D has the range of 0–L, and the ratio r is defined as D/L. In most cases, the previous studies mainly looked at the influence of the arrayperiodicity on the optical performance [10, 12–14]. However, in this letter, the period length L is connected with the density of SiNR arrays ρ and the relationship between them can be derived as $L = (1/\rho)^{1/2}$ ($f_1 = \pi r^2/4$) for square arrays and $L = \left(2/\sqrt{3}\right)^{1/2}(1/\rho)^{1/2}$ ($f_1 = \sqrt{3}\pi r^2/6$) for hexagonal arrays, as shown in Fig. 1b. Obviously, there are three main parameters to be considered: the density of SiNR arrays ρ, the diameter D and length h of SiNR arrays. First, we postulated the density of SiNR arrays as $1.0 \times 10^{10}\,\mathrm{cm^{-2}}$, and later we will verify that the optimal geometric parameters are independent of the array density.

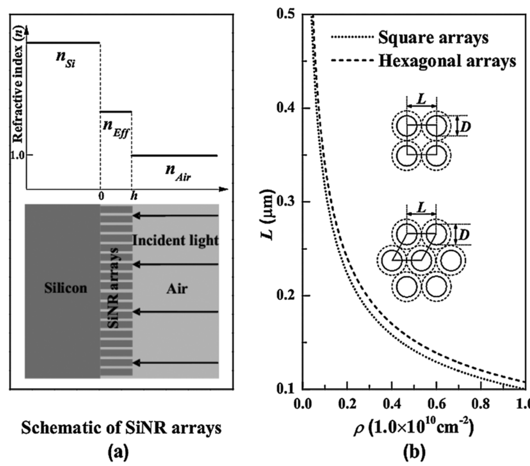


Figure 1 Structure model of SiNR arrays on the silicon substrate. (a) The top part is the distribution of refractive index (n_Si, n_EFF, and n_Air are the refractive index corresponding to the silicon substrate, the SiNR arrays and air, respectively), and the lower part is the profile of SiNR arrays. (b) Graph of period length vs. the array density of the square and hexagonal alignments. The insets are the planforms of different SiNR arrays alignments.

3 Results and discussion The square arrays are first taken into consideration. The ratio r has a big influence on QE and therefore, for different lengths of SiNR arrays, the influence of the ratio r on QE is studied, as shown in Fig. 2. Obviously, for the different lengths of SiNR arrays, there is an optimum ratio r corresponding to the respective maximum QE. Overall, the different peaks of QE fluctuate near 0.72, and the fluctuation range is similar to that from a previous study that reported it is greater than 0.5 [13]. In particular, when r is 0.72 and the length of SiNR arrays is 0.090 μm, the QE is the highest, about 92.4% better than the results from previous studies [20, 21], and the optimum volume filling ratio is about 40.7%.

Taking the length of SiNR arrays as 0.090 μm, the changing curve of QE under the different values of r is shown in Fig. 3. It can be observed that QE reaches its maximum at point b, about 92.4%, where the ratio r is 0.72. Here, the distribution curves of RPF under three typical r values are shown in the inset of Fig. 3 and the shaded area is the total number of reflected photons. From the figure, it is obvious that the shaded area of inset b is the smallest. We can deduce from the contour profile of RPF, that if the SiNR diameter is too small, which means that the air interspaces

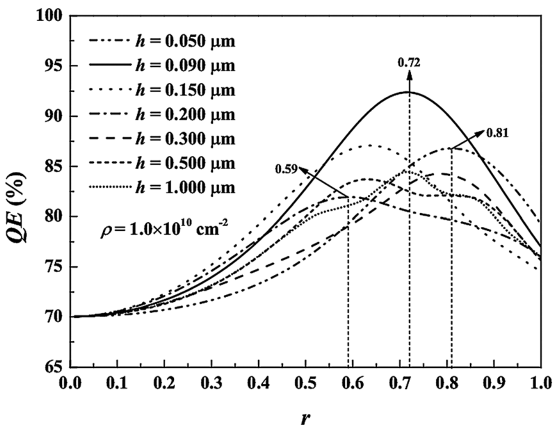


Figure 2 Graph showing how QE varies with the increasing value of r under $\rho = 1.0 \times 10^{10}\,\text{cm}^{-2}$ with different lengths of SiNPs arrays ($h = 0.050\,\mu$m, $0.090\,\mu$m, $0.150\,\mu$m, $0.200\,\mu$m, $0.300\,\mu$m, $0.500\,\mu$m, and $1.000\,\mu$m). The optimum value of r is 0.59, 0.72, and 0.81 corresponding to $h = 0.200\,\mu$m, $h = 0.090\,\mu$m, and $h = 0.050\,\mu$m, respectively.

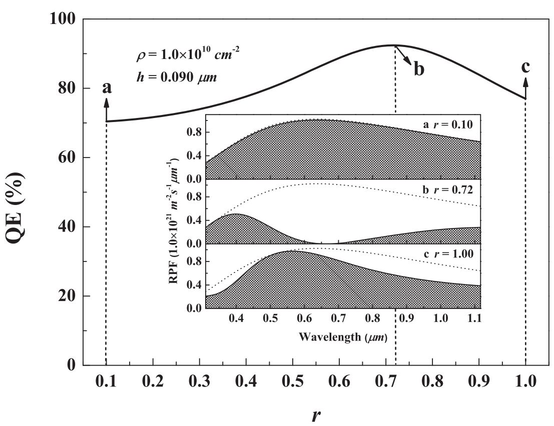


Figure 3 Graph showing how QE varies with the increasing value of r under $\rho = 1.0 \times 10^{10}\,\text{cm}^{-2}$ and $h = 0.090\,\mu$m. The inset is the RPF under different values of r (a, b, and c correspond to $r = 0.10$, $r = 0.72$, and $r = 1.00$, respectively, and the dotted line is the RPF of crystalline silicon).

are too wide, it will result in most of the photons arriving at the surface of substrate easily and being reflected directly. In this case, the RPF is almost as big as that of bare silicon shown at point a where the ratio r is 0.10. On the other hand, if the SiNR diameter is too big, which means that the air interspaces are too narrow, this also leads to bigger RPF. On this occasion, a small number of photons are scattered and captured, but most of them are reflected directly by the top of the SiNR arrays, so the RPF is also bigger, as shown at point c, where the ratio r is 1.00. In short, only under the optimum diameter, can the majority of photons enter the air interspaces and be scattered and captured, which directly results in the RPF of some wavelengths falling to the minimum, especially in the visible light region, as shown at point b.

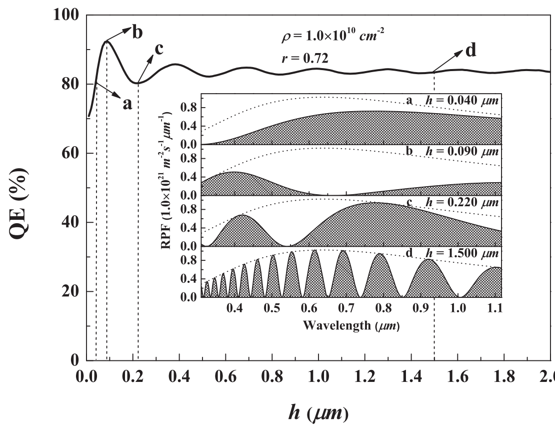


Figure 4 Graph showing how QE varies with the increasing length of SiNR arrays under $\rho = 1.0 \times 10^{10}\,\text{cm}^{-2}$ and $r = 0.72$. The inset is the RPF under different lengths of SiNR arrays (a, b, c, and d correspond to $h = 0.040\,\mu$m, $h = 0.090\,\mu$m, $h = 0.220\,\mu$m, and $h = 1.500\,\mu$m, respectively. The dotted line is the RPF of crystalline silicon).

With the optimal ratio unchanged under the given density, the effect of different lengths of SiNR arrays on QE has been studied, as shown in Fig. 4. It can be seen that QE is an oscillating curve and shows a tendency toward stabilization. It reaches the maximum at point b, about 92.4%, where the length of SiNR arrays is $0.090\,\mu$m. The distribution curves of RPF under four typical length values are shown in the inset of Fig. 4 and the total number of reflected photons is also shown as the shaded area. From the contour profile of RPF, it can be inferred that if the length of the SiNR arrays is too short, most of the photons would be reflected by the surface, with little light-trapping effect. Therefore, RPF is almost as big as that of the bare silicon, as shown at point a where the length of SiNR arrays is $0.040\,\mu$m or less. If the SiNR arrays are longer, some of the photons, which should have been absorbed by the surface of silicon substrate, will be reflected by the SiNR arrays to a certain extent. Therefore, RPF also becomes bigger, as shown at point c where the length of the SiNR arrays is $0.220\,\mu$m. As the length increases, there is very little change in RPF and QE is also almost constant and close to 84.4% as shown at point d, which means that longer SiNR arrays do not lead to more light reflection. With regard to the light-reflection properties, longer SiNWs do not have a positive correlation with the efficiency of solar cells [19, 21]. Only at the optimum length do both the SiNR arrays and the silicon substrate absorb more different energy photons, and at this instance, QE increases to a maximum, as shown at point b.

The 3D relationship among the ratio r, the length of SiNR arrays h, and QE under the given density is shown in Fig. 5. It is evident that there is a maximum QE of 92.4% where r is 0.72 and the length of SiNR arrays is $0.090\,\mu$m. Both the peak value of QE and optimum ratio r fluctuates with the increased length of the SiNR arrays, and finally, the QE is close to 84.4% and the ratio r is close to 0.72. Furthermore, the effects of different SiNR array densities on

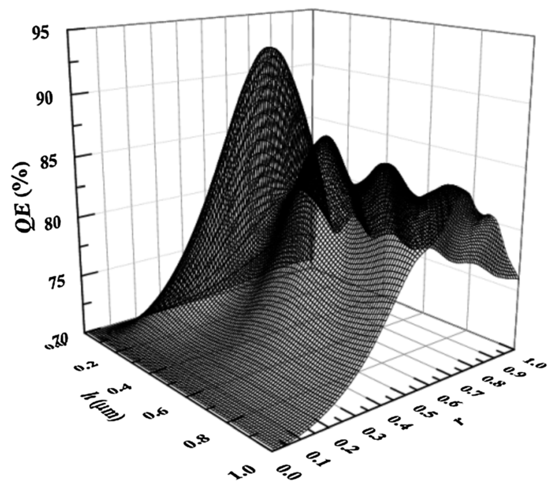


Figure 5 Three-dimensional map of QE versus different lengths of SiNR arrays and values of r under the given array density.

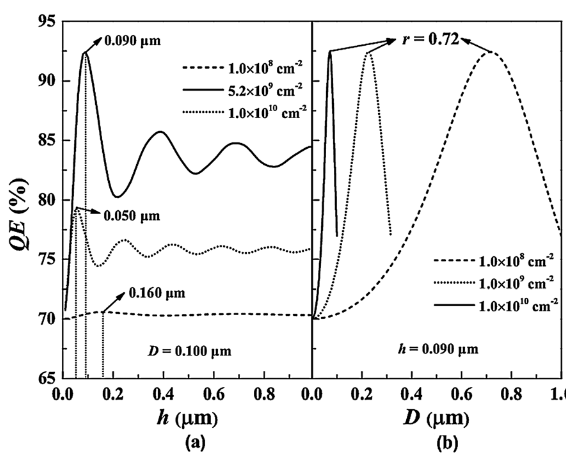


Figure 6 Graphs of QE under the different arrays densities: (a) constant diameter of SiNR, (b) constant length of SiNR.

QE are studied, as shown in Fig. 6. With the SiNR diameter unchanged, which is 0.100 μm, it is found that there is a respective maximum QE under the different densities, as shown in Fig. 6a. First, it shows that the higher density does not lead to better light-reflection property [15]. The best density is $5.2 \times 10^9\,\mathrm{cm}^{-2}$ for the 0.100-μm SiNR diameter that makes the ratio $r = 0.72$. Secondly, the optimum length begins to reduce with the increase in array density for the optimal light-reflection property. It is 0.160 μm for $1.0 \times 10^8\,\mathrm{cm}^{-2}$, 0.090 μm for $5.2 \times 10^9\,\mathrm{cm}^{-2}$, and 0.050 μm for $1.0 \times 10^{10}\,\mathrm{cm}^{-2}$, and the best length is also 0.090 μm corresponding to the highest QE. In the same way, with the length of SiNR arrays unchanged, which is 0.090 μm, it is found that the optimum ratio r is 0.72, which is the same value as that for different array densities for the highest QE, as shown in Fig. 6b.

Comparing the results, it is concluded that when the ratio r is 0.72, the length of SiNR arrays is 0.09 μm, the highest QE of 92.4% is achieved, and it is independent of the array density. In addition, for the hexagonal arrays, the results show that the conclusion is the same except the optimum ratio r is 0.67, which has also been reported in previous studies [22]. For the two types of arrays, the interesting thing is that for the highest QE, under the same array density, both SiNR diameters and lengths are equal despite the different array alignments and optimum values of ratio r. The two arrays have little effect on the resulting light-reflection capability under the same array density, which validates the previous views [8].

4 Conclusions In conclusion, by considering the effect of the diameter and length of semiconductor nanorod on QE, as a typical example, we calculated the performance of the light reflection of SiNR arrays based on the silicon substrate. The results show that the optimal geometric parameters of regular vertical SiNR arrays can be attributed to the minimum number of reflected photons as the shade area of RPF shows. For the SiNR-based solar cells, at any density, although there are optimal geometric parameters to reduce the light reflection, the minimum light reflection occurs at an optimum ratio r of 0.72 for square arrays and 0.67 for hexagonal arrays and the same optimum SiNR length of 0.090 μm. The results show that the optimal design structure of SiNR arrays has a higher QE and is helpful in the design of efficient photovoltaic devices.

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