

Efficient light trapping in silicon inclined nanohole arrays for photovoltaic applications



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ABSTRACT

Structural design with high light absorption is the key challenge for thin film solar cells because of its poor absorption. In this paper, the light-trapping performance of silicon inclined nanohole arrays is systematically studied. The finite difference time domain method is used to calculate the optical absorption of different inclination angles in different periods and diameters. The results indicate that the inclined nanoholes with inclination angles between 5° and 45° demonstrate greater light-trapping ability than their counterparts of the vertical nanoholes, and they also show that by choosing the optimal parameters for the inclined nanoholes, a 31.2 mA/cm² short circuit photocurrent density could be achieved, which is 10.25% higher than the best vertical nanohole system and 105.26% higher than bare silicon with a thickness of 2330 nm. The design principle proposed in this work gives a guideline for choosing reasonable parameters in the application of solar cells.

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1. Introduction

With possible future shortage of energy resources and environmental concerns, a growing interest has been raised in solar photovoltaic technology in recent decades [1]. As a prevailing solar cell material, silicon has several advantages, including lack of toxicity, nearly ideal band gap, high crust abundance, high stability, and compatibility with mature integrated-circuit fabrication techniques [1,2]. However, c-Si is an indirect band gap material such that solar cells are typically several hundred microns thick to ensure high spectral absorption [2]. This results in expensive material costs, not only from the amount of material, but also from high purity requirements to ensure good collection of photogenerated carriers. Thin-film solar cells have emerged as an alternative to reduce material costs and may be suitable for incorporation into low-cost and flexible substrates. In thin-film solar cells, light trapping is important for ensuring high absorption within little photoactive material. Research on light trapping has been burgeoning in the past decade, with both theoretical studies on the limits of absorption enhancement in weak absorbers and experimental demonstrations of a myriad of strategies.

Various structures have been shown to increase the light absorption in the photoactive region, such as plasmonic metal nanostructures [2–7], pyramid structure [8,9], dielectric nanostructure [10–14], photonic crystals [15], diffraction grating [16], and directly nanopatterning the photoactive materials into arrays of nanowires (NWs) [17–22], nanoholes (NHs) [23–30], nanocones (NCs) [31], or nano-cone-holes (NCHs) [32]. Recently, Xu et al. systematically investigated the absorption of Si inclined nanowire arrays with different inclination angles and showed that the optimal inclined nanowire arrays show greater light-trapping ability than their vertical nanowires counterparts [22]. On the other hand, Han et al. showed that nanohole arrays demonstrate great light absorption performance superior to nanorod arrays [23]. Thus, Si inclined nanohole (INH) arrays may show better trapping performance than vertical nanohole arrays. With further investigation, Hong et al. had proposed the structure of inclined nanohole (INH) and have also demonstrated improved light absorption with a fixed inclination. He also illustrated that by controlling the etching solution concentration, the inclined silicon nanohole arrays can be successfully fabricated [25]. Additionally, Liu et al. demonstrated a novel, simple,

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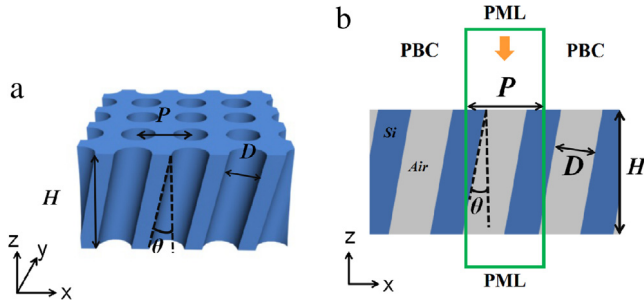


Fig. 1. (a) 3D diagram of silicon inclined nanohole arrays. (b) Schematic of the FDTD simulation model. PML perfectly matched layer, PBC periodic boundary condition.

and low-cost method to fabricate silicon nanohole (SiNH) arrays based on a thin silver film dewetting process combined with metal-assisted chemical etching [33]. Even though Si inclined nanohole arrays are obtained [25,26], the optical absorption characteristics in the solar spectrum of Si inclined nanohole arrays with different inclination angles remain unclear so far.

In this paper, through careful examination of the absorbing capability of INHs with different inclination angles, the results indicate that the inclined nanoholes with inclination angles between 5° and 45° have greater light-trapping ability than their vertical nanoholes counterparts. Moreover, the period and diameters of the NHs have been extensively studied in order to maximize the light absorption of the new system. A 31.2 mA/cm^2 short circuit photocurrent density could be achieved, which is 10.25% higher than the best vertical nanohole system and 105.26% higher than bare silicon with a thickness of 2330 nm.

2. Methods

Fig. 1(a) and (b) show the schematic of silicon solar cells with inclined holes filled by air. The geometrical parameters have been inserted into the figure. The period (lattice constant) of the square lattice is indicated as P . The diameter of the air hole is D , and the thickness is H . The filling ratio (f) of nanostructures is defined as $f = 1 - \pi D^2/4P^2$ [30]. For all simulations in this work, the thickness of the silicon layer is fixed at $2.33 \mu\text{m}$ for a fair comparison with those of [28,30]. All results were numerically simulated based on the finite difference time domain (FDTD) method. In this work, two simulations under illumination polarized in the x and y directions are required with orthogonal polarizations in order to get unpolarized results due to solar light being unpolarized. A plane-wave light with a wavelength range of 300–1100 nm was normally incident. Periodic boundary conditions were adopted in the x and y directions, and a perfectly matched layer boundary condition was used in the z direction. The optical constants for all the media studied in this work were from Palik's experimental data provided in [34]. The p-type and n-type regions are assumed to be lightly doped so that they can be modeled using the same optical constants as intrinsic crystalline silicon. For all simulations, the light reflectance $R(\lambda)$ at the front surface of the cell and the light transmittance $T(\lambda)$ at the rear surface were measured, and the absorptance was determined by $A(\lambda) = 1 - R(\lambda) - T(\lambda)$. Assuming that all electron-hole pair contributes to photocurrent, the short circuit current density J_{sc} is given by [35]

$$J_{sc} = \frac{e}{hc} \int_{310}^{\lambda_g} I_{AM1.5}(\lambda) A(\lambda) \lambda d\lambda \quad (1)$$

where e is the electron charge, c is the speed of light in vacuum, h is the Planck constant, λ_g is the free space wavelength corresponding to the band gap of c-Si ($E_g = 1.12 \text{ eV}$), i.e. 1127 nm, and $I_{AM1.5}(\lambda)$ is the solar irradiance under the global 37° tilt Air Mass 1.5 spectrum [36].

In order to quantify the improvement of the light absorption in nanohole arrays across the solar spectrum relative to the bare silicon

with a thickness of 2330 nm, absorption enhancement factor G is introduced and defined as

$$G = \frac{J_{sc_NH}}{J_{sc_2330nm}} = \frac{\int_{310}^{\lambda_g} I_{AM1.5}(\lambda) A_{NH}(\lambda) \lambda d\lambda}{\int_{310}^{\lambda_g} I_{AM1.5}(\lambda) A_{2330nm}(\lambda) \lambda d\lambda} \quad (2)$$

3. Results and discussion

In order to facilitate comparison and illustrate the correctness of the method, we first studied the short circuit current density of 2330 nm bare c-Si film and the optimal absorption enhancement G of silicon vertical nanohole arrays with different periods and different filling ratios for reference. The short circuit current density of 2330 nm bare c-Si film is $J_{sc} = 15.2 \text{ mA cm}^{-2}$ based on Eq. (1). Fig. 2 shows the dependence of the absorption enhancement G of square lattice crystalline silicon nanostructures on the period (P) and the filling ratio for the normal incidence. Periods is varied from 400 nm to 800 nm with 100 nm intervals while filling ratios is varied from 0.3 to 0.8. According to Ref. [30], the optimal period and filling ratio (f) of the vertical nanoholes are about 600 nm and 0.54, respectively, so the period is limited from 400 nm to 800 nm. In this work, we found the optimum result occurs at $P = 600 \text{ nm}$ and $f = 0.54$, which is close to that reported in Ref. [30]. The absorption enhancement is $G = 1.86$ and the shortcircuit current density is $J_{sc} = 28.3 \text{ mA cm}^{-2}$ in this case. The results of the following research will compare with this optimal shortcircuit current density.

3.1. The effect of inclination angle

The averaged absorption spectra of Si nanohole arrays with different inclination angles and the absorption enhancement with different inclination angles are shown in Fig. 3. The period and diameter of the NH are fixed at 600 nm and 480 nm, respectively, the same with the optimal parameters of the vertical nanoholes. Referring to Fig. 3(a), Si nanohole arrays show an obvious advantage against the bare Si in all wavelength regions due to the light-trapping properties and antireflection effect of NH arrays. Additionally, the inclined nanohole arrays achieve better light absorption than the vertical nanohole arrays ($\theta = 0^\circ$) from wavelength 580 to 800 nm. Furthermore, the absorption has no apparent discrepancy from wavelength 380 to 550 nm, while in the wavelength region less than 380 nm, the light-trapping performance improves with the increase of the inclination. This shows that the size of the hole rises with increasing angle inclination and that nanoholes with these large holes show higher light absorption in the short wavelength, which is in accord with the conclusion of Zhang et al. [28]. Peaks in absorptivity spectra can be attributed to the essential mechanisms such as wave interference, Bloch resonance modes and coupling effects [6,30].

To better understand the behavior of the inclined nanohole arrays, the absorption enhancement with different inclination angles for x and y polarizations are shown in Fig. 3(b). The inclination angles vary from 0° to 70° with an interval of 5° . It is obvious that the absorption enhancements for y polarizations are greater than x polarizations from an inclined angle 10° to 50° . It shows that this unique geometry is more sensitive under y polarization. At the same time, there is a spike in absorption enhancement of 2.12 for y polarization when the inclination is 25° and the optimal inclination for x polarization is 10° . To simulate the absorption enhancement of solar light, we take the average of x polarization and y polarization. Because the absorption in the short-wavelength region is enhanced with the increase of inclination angles while it is decreased in the long-wavelength region with the increase of inclination angles. The increments and reductions get to a trade off when the inclination is 25° . So an optimal average absorption enhancement of 2.02 is achieved at this inclined angle. The shortcircuit current density is $J_{sc} = 30.7 \text{ mA cm}^{-2}$ in this case, which is 8.48% and 101.97% higher than the best vertical nanohole structure counterpart, the bare silicon with a thickness of 2330 nm, respectively. This result

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