

Characterization of light absorption in thin-film silicon with periodic nanohole arrays

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Abstract: Light absorption in thin-film nanostructured monocrystalline silicon (c-Si) in a glass/Ag(0.2 μm)/c-Si(1 μm) stack is characterized using simulations and measurements. Nanohole (NH) arrays designed for a practical thin-film solar cell configuration experimentally exhibit a significant improvement of the light absorption in the 1- μm ultrathin c-Si layer that exceeds the theoretical Yablonovitch limit in the long wavelength range. Fabricated square-lattice and hexagonal NH arrays give relative improvements of 65 and 70%, respectively, in the total absorption compared to a nonpatterned stack. The effect of an indium-tin-oxide (ITO) coating is also simulated, and an empty NH configuration gives the lowest ITO parasitic absorption.

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1. Introduction

Thin-film solar cells not only require less material for fabrication but also have a higher photocarrier concentration with less bulk recombination in the active layer compared to bulk crystal solar cells [1]. However, the light absorption depth in silicon is significantly longer at photon energies close to the band gap resulting in low absorption and therefore low efficiency.

To achieve better light absorption performance, several approaches such as diffraction gratings, photonic crystals, and metal nanoparticles [2–4] on the front or back surface of the solar cell have been introduced. Texturing the cell active layer with nanostructures has also been theoretically demonstrated to improve the possibility of enhancing the absorption [5–8]. Periodic high-aspect-ratio nanorod arrays with skewed pyramids exceed the Yablonovitch limit over a broad wavelength range [6], and periodic nanohole (NH) arrays exhibits better absorption than periodic nanorod arrays [9]. Motivated by these theoretical studies, the practical implementation of nanostructures in thin-film solar cells and its experimental verification has become an intriguing subject. Current silicon technology allows the low-cost fabrication of NH arrays over a large area with precise dimensions [10–12]. Experimental studies of periodic NH arrays on thick monocrystalline silicon (c-Si) solar cells have been reported [13–16]. Periodic NH arrays on thick silicon wafers reduce the reflection of broadband sunlight wavelengths [16] and increase the solar cell efficiency by 19% relative to nonpatterned silicon [14]. These experimental studies suggest the great potential of periodic NH arrays to enhance the light absorption of thinner thin-film c-Si solar cells. Studies focusing on absorption enhancement in ultrathin c-Si solar cells (e.g. <3 μm thickness) with periodic NH arrays have been reported [7, 17–21], but, to the date, few have reported

experimental results [17, 19]. In addition, periodic NH geometry optimization has tended to be carried out using a rather simplified model and method.

In this paper, further investigation of the light absorption enhancement of periodic NH arrays on a 1- μm ultrathin c-Si film with a silver back reflector was carried out to experimentally verify the optical performance with the aim of using these films in solar cell applications. We first optimize the NH array geometry and simulate the expected light absorption in the c-Si active layer by a 3D full-field finite difference time domain (FDTD) calculation using parallel supercomputing. Optical measurements of the optimized array geometry are then performed, and we examine the effects of different transparent conductive oxide (TCO) layer configurations.

2. Simulation model and methodology

Figure 1 shows a schematic diagram of a periodic NH array with the Ag back reflector; Ag is preferred due to its low loss characteristics [22]. The design parameters to be optimized are the lattice constant P and filling factor ff , defined as the volume ratio of air to one unit cell. The NH diameter is denoted by D . The NH depth h , thickness of the Ag back reflector, and c-Si layer thickness were fixed at 500 nm, 200 nm, and 1 μm , respectively.

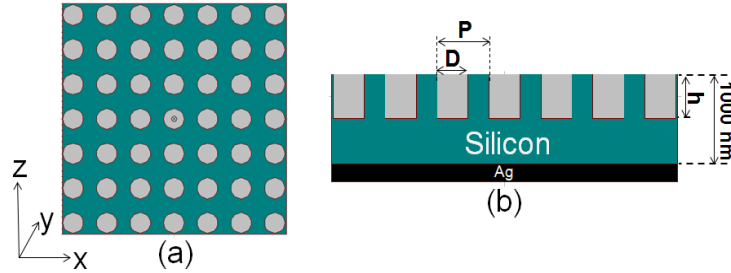


Fig. 1. Schematic of the c-Si NH arrays: (a) top view and (b) side view.

The spectral absorption characteristics of the proposed model were investigated by performing 3D full-field FDTD calculations using high-performance parallel supercomputing. The optical properties of Ag, c-Si, and indium-tin-oxide (ITO) were taken from the literature [23, 24]. Periodic boundary conditions were enforced in the x and z directions, while a perfectly matched layer (PML) boundary condition was applied in the y direction. Light was incident normal to the surface.

The total absorption in the c-Si layer can be expressed as

$$\alpha(\lambda) = \frac{\omega}{2} \int_V \text{Im}[\varepsilon(\omega)] |E(t)|^2 dV, \quad (1)$$

where E is the electric field, ε is the spatially dependent permittivity, and dV is the finite volume in the monitored volume V . According to theory describing the light to current conversion, the enhancement in the total light absorption can be quantified by the improvement in the short circuit current density. By assuming that each photon absorbed in the c-Si layer generates an electron-hole pair, the short circuit current density can be calculated as

$$J_{sc} = e \int_{300}^{1100} \alpha(\lambda) S(\lambda) d\lambda, \quad (2)$$

where e is the electron charge, $\alpha(\lambda)$ is the optical absorption, λ is the wavelength, and $S(\lambda)$ is the incident solar photon flux density from an air mass (AM) 1.5 G standard spectrum.

3. Results and discussion

3.1 Optimization of the NH array geometry and comparison with perfect geometrical light trapping

The optimization was performed to maximize J_{sc} in the c-Si, that is, the active layer of a solar cell. The J_{sc} values for different P and ff combinations were compared. The maximum J_{sc} occurs at $ff = 0.25$ for $300 \text{ nm} \leq P \leq 600 \text{ nm}$, and $P = 600 \text{ nm}$ gives the highest J_{sc} value. For this P and ff combination, the effect of the NH depth h on J_{sc} is investigated for $300 \text{ nm} \leq h \leq 900 \text{ nm}$. Consequently, $h = 500 \text{ nm}$ gives the highest J_{sc} value of around 130 A/m^2 . It should be noted that, in general, surface recombination, which is not considered in the present J_{sc} calculation model, increases as the surface area increases, and hence degrades the conversion efficiency [25]. That is, in an actual thin-film NH solar cell, the best NH depth could be different from the present optimized depth.

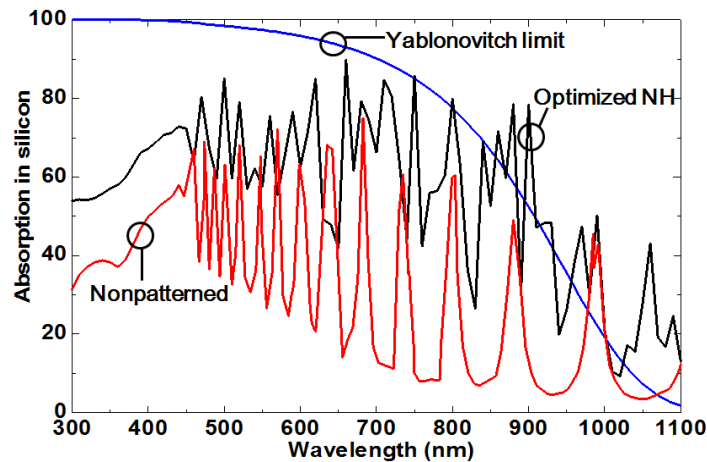


Fig. 2. Absorption spectra for the optimized c-Si NH array ($P = 600 \text{ nm}$, $ff = 0.25$, $h = 500 \text{ nm}$) with a Ag back reflector compared to a nonpatterned c-Si with Ag back reflector, and the Yablonovitch limit. The incident angle is normal to the surface.

Figure 2 shows the spectral absorption in c-Si for the optimized NH geometry ($P = 600 \text{ nm}$, $ff = 0.25$, $h = 500 \text{ nm}$). For comparison, the spectral absorption in a nonpatterned c-Si as well as the Yablonovitch limit (the theoretical limit of perfect geometrical light trapping [26]) are also shown. The NH array exhibits a higher absorption spectrum than the nonpatterned c-Si over the simulated spectrum range. The absorption enhancement seen in the short wavelength region is expected from the antireflective effect in which incident light sees the surface having a continuous refractive index gradient between air and the silicon [9]. However, in this short wavelength region, the NH array is unable to reach the Yablonovitch limit. In the longer wavelength region, the NH array absorption spectra shows absorption peaks with a complex, irregular shape. The absorption enhancement in this wavelength range could be expected from diffraction trapping of incident light [9] and resonant modes [27] attributed to the NH array. Several additional peaks caused by resonant modes can be observed in this wavelength range through a comparison with the nonpatterned c-Si. Some peaks exceed the Yablonovitch limit in the region where silicon is typically a poor absorber. These results support the recent literature emphasizing that NH arrays have a potentially good light trapping performance for thin-film silicon and consequently may contribute to efficiency enhancement in thin-film solar cells. Hereafter, “total absorption” refers to the integrated absorption weighted by a normalized AM1.5G standard spectrum. An increase of 100% relative to the nonpatterned c-Si was achieved.

3.2 Optical measurement of fabricated NH arrays

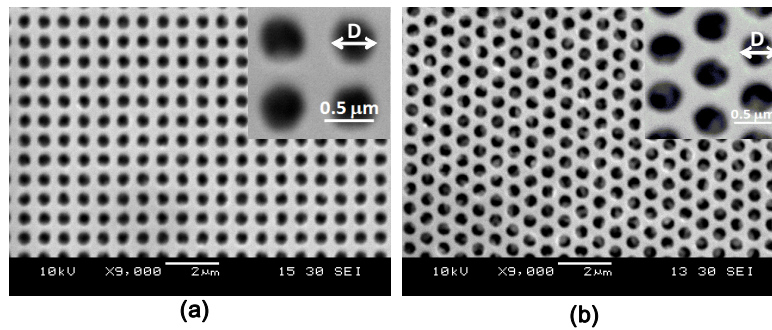


Fig. 3. SEM images of the fabricated (a) square-lattice and (b) hexagonal NH arrays on c-Si.

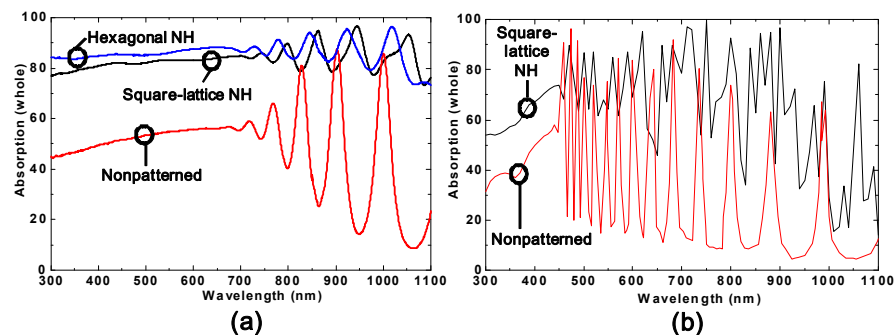


Fig. 4. Comparison of the (a) measured and (b) simulated absorption spectra of a whole stack.

NH arrays were fabricated with the optimized design parameters. A 1- μm thick c-Si layer was fabricated on a silica glass substrate using magnetron sputtering, and the NH arrays were formed using an electron beam lithography technique and plasma etching. Both square-lattice and hexagonal NH arrays were fabricated, since hexagonal NH arrays on a “thick” (1 mm) c-Si wafer were shown in our previous study to have good absorption enhancement properties. A nonpatterned c-Si sample with the same dimensions was also fabricated as a reference. Figure 3 shows scanning electron microscope (SEM) images of the fabricated samples. The average NH depth measured using 3D laser scanning microscope (KEYENCE VK-X200) is approximately 470 nm. The reflectance measurements were performed using a ultraviolet-visible/near-infrared (UV-VIS/NIR) microscopic spectrophotometer (JASCO MSV-5200), which has a Cassegrain reflector that directs monochromatic light to the sample surface within a 23° incident angle of the normal and detects light reflected from the sample surface within the same 23° angle. The measurements were taken for wavelengths of 300 to 1100 nm in 0.5 nm steps, and the absorption of the whole stack was derived from $\text{Abs}(\lambda) = 1 - \text{Ref}(\lambda) - \text{Trans}(\lambda)$, where $\text{Ref}(\lambda)$ and $\text{Trans}(\lambda)$ are the reflection and transmission, respectively.

Figure 4 shows the measured and simulated absorption spectra of the NH arrays and the nonpatterned c-Si. The measured absorption of the NH arrays (Fig. 4(a)) shows remarkably higher values compared to the nonpatterned case as predicted by the simulations. However, the simulation showed more absorption peaks and a slightly lower absorption over the wavelength range than that seen in the measurement data. This could be caused mainly by the difference in the incident and detected angles in the measurement and simulation. In the measurement, the reflectance was observed as integrated reflectance within the 23° incident and detected angles and thus rapid fluctuations compensated each other, whereas in the simulation, the reflectance was obtained as hemispherical-integrated reflectance based on only the normal incidence. In addition, defects such as roughness, etched slopes, and a nonconstant

ff could not be avoided in fabrication; these could also be responsible for a compensation of the rapid fluctuations. The measured relative improvements of the total absorption for the square-lattice and hexagonal NH arrays to the nonpatterned c-Si are 65 and 70%, which is a 7% improvement of that recently reported for the same silicon thickness [17].

3.3 Effect of ITO layer on NH arrays

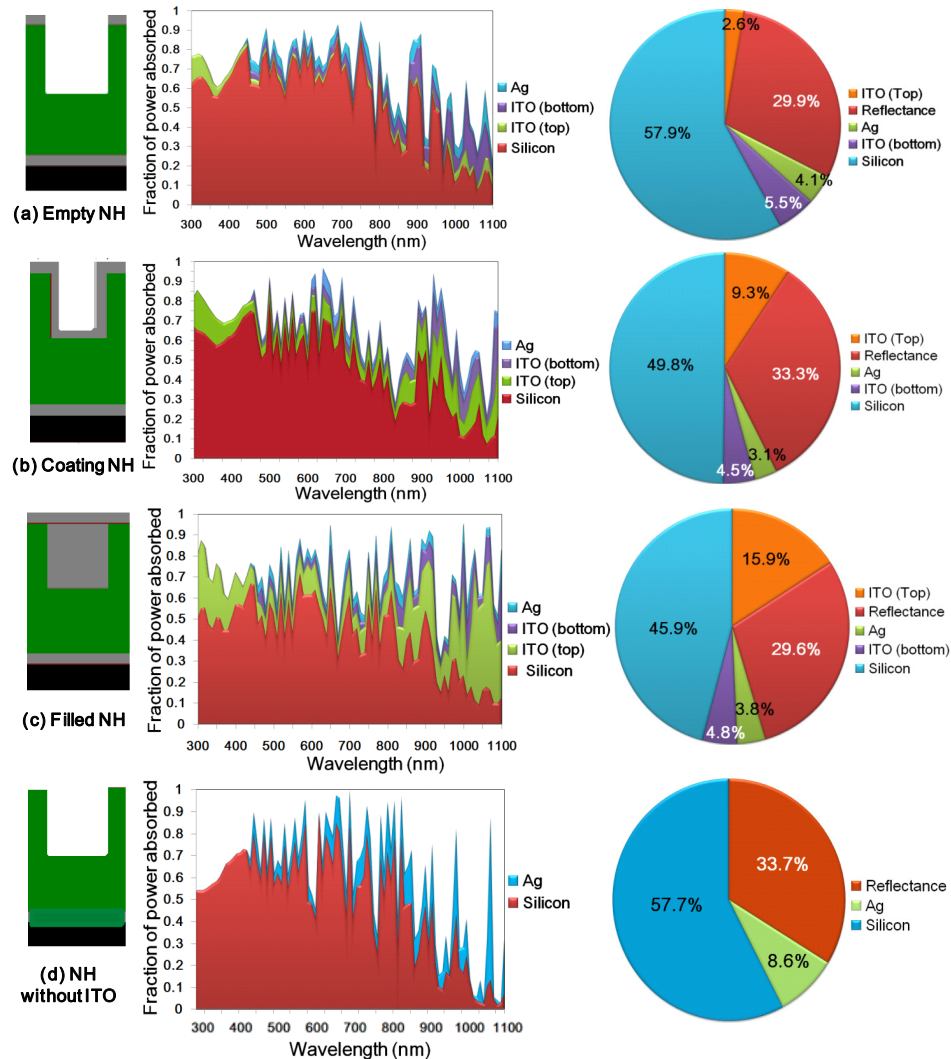


Fig. 5. (left) Three possible ITO layer configurations, (middle) calculated absorption in each layer of the stack, and (right) the total absorption and reflection percentages in each layer of the stack; (a) empty NH, (b) coated NH, (c) filled NH, and (d) NH without ITO. Optimized parameters for the square-lattice c-Si NH arrays are used for every configuration.

Introducing a transparent conductive oxide (TCO) layer into the solar cell will provide an antireflection effect contributed by the refractive index gradient at the TCO–c-Si interface and will reduce reflection losses. However, a portion of the trapped light can be absorbed by the TCO layer. This parasitic absorption will be counterproductive to improving the light absorption in the c-Si layer and the conversion efficiency. Therefore, it is important to investigate the effect of a TCO layer on the absorption spectrum. Here, ITO was selected as the TCO because of its suitable properties for thin-film solar cells [28].

Three possible top ITO layer configurations were modeled: an empty NH, a coated NH, and a filled NH as shown in Fig. 5 (left). The ITO layer was 85 nm thick, except in the case of the filled NH. This thickness has been reported to give the minimum reflectance [29]. Figure 5 (middle) shows the fraction of power absorbed in each layer of the whole stack. As expected, the empty NH shows the highest absorption in the c-Si layer and the filled NH shows the lowest. In the short wavelength range (<450 nm), a substantial part of the incident light is absorbed by the top ITO layer for all configurations because at this wavelength range, the ITO extinction coefficient is relatively high. With the filled NH, the absorption in the c-Si is considerably decreased due to the excess volume of ITO. In the longer wavelength range (>450 nm), the best case with the empty NH shows that the absorption in the top ITO layer remained low, but the absorption in the bottom ITO layer is slightly higher than that in the top ITO layer. A small amount of absorption loss occurs in the Ag back reflector. However, for the worse case with the filled NH, severe parasitic absorption occurs in the top ITO layer.

Figure 5 (right) shows the resulting total absorption and reflection percentages for each ITO configuration. Only the empty NH retains an approximately similar total absorption in c-Si (57.9% as compared to 57.7%). The coated and filled NH arrays decrease the absorption to 49.8 and 45.9%, respectively. Parasitic absorption in the top ITO layer is correlated to the ITO volume and accounted for 2.6, 9.3, and 15.9% in the empty, coated, and filled NH arrays, respectively. Absorption in the Ag layer and bottom ITO are very similar in all cases. Consequently, in terms of optical characterization, an empty NH array appears to be the best configuration. These results imply that investigating only the reflectance of the whole stack is not enough for evaluating the absorption in the c-Si layer. Furthermore, it should be noted that the above discussion is limited to the optical behavior of ITO. The electrical behavior of ITO also can play an important role in electron transport. Of these three configurations, the coated NH array may have the added advantage of fast electron transport.

4. Conclusion

Improvement of the light absorption in periodic NH arrays on 1- μ m ultrathin c-Si with a Ag back reflector has been characterized through optical simulations and measurements. The simulation results show a relative improvement of 100% in the total absorption in the c-Si layer compared to nonpatterned c-Si. A stack fabricated with an optimized geometry shows a relative improvement of the total absorption in the whole stack of 65–70% compared to a nonpatterned stack. Owing to the parallel-supercomputing optimization, these improvements currently represent the best experimentally measured results for 1- μ m ultrathin c-Si NH arrays with a back reflector. Through investigations of different ITO configurations, an empty NH pattern was revealed to produce the lowest parasitic absorption of 2.6% in the top ITO layer. The present results support the optical advantages of NH arrays as an excellent thin-film silicon absorber, which implies a good potential for thin-film solar cell applications.