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Towards Perfect Anti-Reflection and Absorption for Nanodome-Array Thin Film Silicon Solar Cell

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Abstract

In this study, a novel nanodome array structure for thin film silicon solar cell is proposed and systematically simulated. This design not only reduces surface recombination, but also achieves a high broadband absorption regardless of the polarisation and incident angles of light, by taking advantage of almost perfect anti-reflection, Mie scattering and Fabry-Perot resonance. The fabrication of such a nanodome structure is technically feasible and the proposed approach is also applicable to other solar cell materials.

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Keywords: Nanodome; antireflection; solar cell; resonance; light absorption

1. Introduction

Photovoltaic is a promising source for future renewable energy. Currently, the commercial market is dominated by crystalline silicon (Si) due to its abundance, nontoxicity and mature technology. However, due to the poor light absorption in Si, an absorbing layer over 200 \( \mu \text{m} \) is required to effectively absorb the sunlight, which accounts for the high cost of Si solar cell [1]. In contrast, thin film solar cells provide an economical alternative by greatly reducing the material required and hence the manufacturing cost. However, it is crucial to improve the photon management ability of thin film solar cells so that high

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power conversion efficiency (PCE) can be achieved. Many studies have focused on incorporating Si nanostructures, like nanowire [2], nanocone [3], and nanopillar [4] arrays, into Si solar cells to enhance light harvesting. They have demonstrated a much reduced light reflection and strong light trapping ability. When the sunlight with a wavelength comparable with the dimension of the nanostructure, strong scattering is induced which effectively prolongates the sunlight optical path length [2-4]. Nevertheless, the large surface area associated with these nanostructures aggravates the surface recombination loss, which in turn substantially degrades the carrier collection efficiency [5]. To address this issue, low aspect ratio nanodome and nano-pyramid Si solar cell structures have been proposed to achieve both efficient light absorption and carrier collection [6-10]. Such structures can improve the device performance by reducing light reflection while enhancing absorption by coupling most of the incident sunlight into the low aspect ratio nanostructures. Furthermore, as the roughness factor, defined as the ratio between the actual surface area and geometric surface area of the structure, is much smaller than that of nanowire, the surface recombination is significantly reduced. Besides, due to the more planar surface, conformal deposition of top electrode can be achieved in contrast to Si nanowires based cells. The nanodome structure has been successfully fabricated and demonstrated the highest short circuit current ever reported among nanostructure based solar cells [7]. Therefore, the novel low aspect ratio nanostructure is a promising and practical approach for light management to boost the PCE of solar cells.

In this paper, we systematically investigate the absorption enhancement mechanisms for poly-Si nanodome structure incorporated with both top amorphous silicon nitride (Si$_3$N$_4$) antireflection coating (ARC) and back silver (Ag) reflector. The top Si$_3$N$_4$ also functions as surface passivation layer to lower carrier recombination. Our simulation results show that the proposed structure can achieve almost perfect antireflection and broadband absorption for both TE and TM polarisations and moreover the performance depends little on the illumination angle.

2. Simulation details

High Frequency Structure Simulator (HFSS) [11] has been used to carry out three-dimensional (3D) Finite Element Method (FEM) simulations to determine the absorption in the nanodome array structure. The basic structure of the nanodome is shown in Fig. 1 with both 3D schematic and cross-sectional views. The structure periodicity is set as P. The thickness of the thin film (T$_2$) is fixed at 1 μm. On top of device is a thin layer of Si$_3$N$_4$ having a thickness of T$_{Si3N4}$, acting as an antireflective layer and passivation layer to reduce the surface recombination. The bottom electrode is 200 nm (T$_3$) thick silver. The light absorbing Si thin film is sandwiched between the two layers. Due to the periodicity, only one unit cell incorporated with periodical boundary conditions is simulated. The top and bottom of the structure are bounded by the

![Fig. 1. The simulated nanodome thin film solar cell structure. (a) 3D schematic and (b) cross-sectional view of the nanodome structure.](image)
Perfectly Matched Layer (PML) [11]. Solar light irradiates the cell from the top with TE and TM polarisation at varying incident angles. To match the solar spectrum to Si absorption, photon energy ($E_f$) ranges from 1.1 eV to 4.2 eV (corresponding to 300 nm to 1130 nm) has been selected. The results are then weighed by the AM 1.5G solar spectrum to get the ultimate efficiency ($\eta$) [6, 12] to facilitate performance comparison. The dielectric constants of the materials used are obtained from the literature [13, 14].

3. Results and discussion

Figure 2 depicts the simulated absorption spectra for the proposed nanodome solar cell with varying P and fixed $T_{Si3N4}$ of 40 nm and the inset plots their $\eta$. It is found that the nanodome structure achieves a high broadband absorption for different P. For light with $E_f$ larger than 1.8 eV, the absorption is approaching 100%, whereas for low $E_f$ light the absorption exhibits oscillation with slight degradation of absorption efficiency. The inset shows the $\eta$ value for the nanodome structure above 35% and with weak dependence on P from 700 nm to 900 nm. This result suggests that a large tolerance is possible in the value of P in the actual fabrication process.

![Absorption spectra of nanodome structure solar cell. The inset shows the ultimate efficiency at different structure periodicity P.](image)

In the following, we will present results for cells with a fixed P of 800 nm. Figure 3a shows the absorption spectra for cells with different $T_{Si3N4}$ and the inset plots their $\eta$. As the thickness increases from 50 nm to 80 nm, the absorption at high $E_f$ degrades while it improves for low $E_f$. The $\eta$ peaks at 36.7% at around $T_{Si3N4} = 70$ nm, attributed to the improved absorption in the range 1.7 eV < $E_f$ < 2.5 eV, which corresponds to the peak of the solar spectrum. Figure 3b depicts the absorption and reflection spectra for the optimised nanodome structure and corresponding pure Si nanodome structure (P = 800 nm, without top $Si_3N_4$ and bottom Ag layers). It is clearly shown that the reflection is significantly reduced and absorption is improved.
Figure 3. (a) Absorption spectra of nanodome structure with different Si$_3$N$_4$ thickness. The inset shows the ultimate efficiency at different Si$_3$N$_4$ thickness. (b) Absorption and reflection spectra of nanodome structure with/without the Si$_3$N$_4$ layer.

Figure 4 shows the normalised electric field (E-field) distribution for the nanodome cell structures at two incident photon energies of 2.48 eV and 1.24 eV and different polarisations. Figure 4a shows the unit cell of the nanodome structure revealing the physical locations of the different layers with the E-field polarised in the x direction. Figures 4b, c, and d plot the corresponding electric field distribution at incident light photon energies of 1.24 and 2.48 eV. Previously, for the Si based thin film solar cells, the absorption is low due to the high reflection from the top surface and incomplete absorption as a result of lack of light trapping features. However, our nanodome structure can effectively suppress those two losses with a much intensified E-field trapped inside the nanodome structure as shown in Figs. 4b, c, and d. For high $E_f = 2.48$ eV, the incident light is absorbed in a single path through the Si layer (Fig. 4b). In the case of illuminating with a low $E_f = 1.24$ eV, light reaches the bottom layer and is then reflected back, efficiently coupled into guiding modes in the Si film in both x and y directions (Fig. 4c, Fig. 4d).

Fig. 4. Normalised electric fields across the cell structure. (a) Unit cell of the nanodome structure, (b) electric field distributions with incident light $E_f = 2.48$ eV in the E$_x$ direction, (c) electric field distributions with incident light $E_f = 1.24$ eV in the E$_x$ direction and (d) in the E$_y$ direction.
Three absorption enhancement mechanisms are identified to be responsible for the observed large and broadband absorption enhancement in our nanodome structure solar cells. The first mechanism is related to the gradual change of refractive index. It has been shown that for an ARC to be effective over a wide range of incident angles, it requires multilayer inhomogeneous coatings with refractive indices that are close to that of the ambient medium [15, 16]. Figure 5 shows the effective refractive index $n_{\text{eff}}$ for the nanodome structure cell as a function of the depth in the cell. The $n_{\text{eff}}$ is defined as the average refractive index between air and nanodome structure based on the volume fraction of each material. The $n_{\text{eff}}$ changes continuously from air into the Si layer, eliminating abrupt interfaces which generally are responsible for large reflection. Hence, with the improved refractive index matching with air, the nanodome structure can effectively suppress light reflection and couple light into the underlying Si layer. The second mechanism is associated with the enhancement due to Mie scattering. Since the feature size of the nanodome structure is comparable with the wavelength of sunlight, it functions as a strong scattering element and supports a large number of diffraction channels. Hence, the nanodome structure can effectively scatter light into different directions, with a sharper and more intense pattern in the forward direction into the Si layer [17]. Therefore, the optical path length is substantially increased resulting in stronger absorption. Furthermore, as the Mie scattering is not strongly wavelength dependent [17], the enhancement in the absorption is broadband. The last mechanism directly relates to the Fabry Perot (FP) resonance. The top ARC layer and bottom Ag reflection layer form a cavity for the resonance. At resonance, the sunlight bounces back and forth within the cavity and enhances the E-field within the Si layer, and consequently results in a stronger absorption [18, 19]. This can be verified from the electrical field distribution within the nanodome structure, where a strong E-field pattern is formed. This is particularly important for long wavelength light ranging from 800 nm to 1100 nm with weak absorption where a single path is not sufficient to substantially absorb the incident light. As shown in Fig. 4.c at $E_f=1.24$ eV, a strong E-field pattern similar to waveguide mode TM$_{11}$[20, 21] is formed with the peak E-field increases by 8.5 times ($[(E/E_0)^2 = 72]$), demonstrating a higher enhancement exceeding the Lambertian limit [19, 22]($4n^2 \approx 50$ for Si, where $n$ is the refractive index of Si).
As the incident sunlight can be very diffuse, it is important to evaluate the sensitivity of the absorption as a function of the polarisation and incident angles of light. Figure 6 show the light absorption spectra and ultimate efficiency respectively as the incident angle varies from 0° to 60° for both TE and TM polarised light. As the incident angle increase from 0° to 60°, the absorption over the whole spectrum for the nanodome structure remains excellent without significant degradation and the ultimate efficiency stays above 34%, still much higher than corresponding pure Si nanodome structure. This is because at the oblique incident angle, the three enhancement mechanisms identified above are still effective. Hence, our nanodome structure demonstrates the ability to realise a broadband and polarisation-insensitive absorption enhancement for practical application of thin film solar cells.

4. Conclusion

In conclusion, a systematical study has been conducted to investigate the absorption characteristics of the nanodome Si thin film solar cell by incorporating the top ARC layer and bottom Ag layer simulate using the finite element method. The light absorption has been found to be substantially improved. Three mechanisms, the gradual change of the refractive index, Mie scattering and Fabry-Petrot resonance, are identified to be responsible for the observed light absorption enhancement. In addition, the proposed nanodome structure achieves a near perfect light absorption that is broadband and insensitive to the polarisation of light and incident angle due to its superior anti-reflection property and strong light harvesting ability. Hence, this structure is promising for the fabrication of high efficiency thin film Si and other types of solar cells.

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Reference