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Optical absorption enhancement of nanoconical frustum arrays texturing for c-Si film solar cells

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ABSTRACT

In this work, we demonstrate silicon thin film with square nanoconical frustum arrays decorated surface via simulation for photovoltaic application. An ultimate efficiency of optimized silicon square nanoconical frustum (SiSNF) arrays based solar cells is up to 31.60%, 3.47% higher than that of silicon thin film based solar cells with silicon hexagonal nanoconical frustum (SiHNF) arrays textured surface, which is close to the perfect Yablonovitch surface. The enhanced ultimate efficiency of SiSNF arrays is insensitive to top diameter and incident light angle. The underlying absorption enhancement mechanism behind the observation is also discussed.

1. Introduction

In recent years, numerous silicon nanostructures, such as nanopore [1,2] nanocone [3–5] and nanowire [6–10] arrays, have attracted many attentions due to their unique physical properties and potential optoelectronic applications, especially the promising candidate for photovoltaic applications thanks to the feasibility to decouple light trapping and photo-generated carrier extraction [11–13]. In addition, nanostructures also enable the use of low purity Si, thus reducing the manufacturing cost. However, the high aspect ratios associated with silicon nanopore [1,2] or nanowire [6–10] arrays potentially affect conformal deposition of transparent electrodes, resulting in poor photo-generated carrier collection, and thus low power conversion efficiencies. As an alternative surface nanostructure for optical absorption enhancement, Silicon square nanoconical frustum (SiSNF) arrays decorated Si film was recently reported to increase the efficiency of Si film based solar cells [14,15]. In addition, the SiSNF arrays have been empirically demonstrated in many groups, which have low aspect ratio as well as the advantage of easy fabrication via Langmuir–Blodgett assembly [16]. However, the detailed simulation parameters regarding to the SiSNF arrays based solar cells have not been reported.

In this paper, SiSNF arrays with low aspect ratios are introduced for Si thin film based solar cells. The thickness (H) of the underlying Si film is fixed to be 800 nm. The other parameters of the proposed structure, such as the period (P) of the square lattice, the top diameter (D_{top}), the bottom diameter (D_{bot}) and the length (L) of SiSNF arrays, are systematically studied via simulation. The results show that the ultimate efficiency as high as 31.60% is achieved when the parameters D_{top}, D_{bot} (equal to P), H, and L are fixed to be 100, 700, 800, and 1000 nm, respectively. In addition, the enhanced ultimate efficiency is insensitive to D_{top} and incidence light angle, which could facilitate the SiSNF arrays in solar cells applications. The underlying physics mechanism behind the observation is also discussed.

2. Method

The Rigorous Coupled Wave Analysis (RCWA) enhanced by the Modal Transmission Line (MTL) theory is employed to simulate the interaction between incident light and the proposed structure, which is realized by infinitely extending the structural unit (shown in Fig. 1(b)). The simulation methodology based on RCWA and MTL has been verified by the report [17–19] and our previous study [20]. The periodic boundary conditions were adopted in x, y directions and a perfectly matched layer boundary condition was used in the z direction in order to let reflected light escape from simulation volume, as shown in Fig. 1(a). The reflection and transmission were calculated first, and then the absorption is

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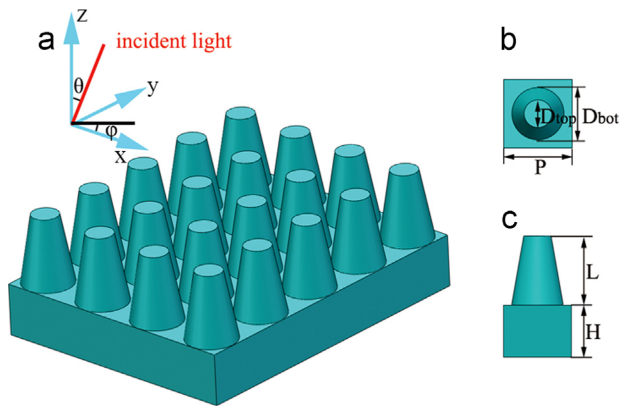

Fig. 1. (a) The schematic 3D drawing of the SiSNF arrays, (b) 2D top view and (c) side view of the structural unit of SiSNF arrays.

given by $A = 1-R-T$. The direction of the incident light is determined by the azimuthal (φ) and zenith (θ) angles. In the following simulation, both azimuthal and zenith angles are fixed to be zero unless otherwise stated. Therefore, the incident light is perpendicularly projected onto the Si film surface with the light energy varied from 1.1 to 4 eV, covering the major solar spectrum in interest, and the polarization direction is parallel to the x axis.

3. Results and discussion

The schematic of the proposed SiSNF arrays textured Si film-based solar cells, and the parameters of the proposed structure, such as P, D_{top}, D_{bot}, and L, are shown in Fig. 1(a)–(c). The thickness (H) of the underlying Si film is fixed to be 800 nm in the z direction. The refractive index (n) and the absorption index (k) used in the simulation refer to crystalline silicon [21]. According to the Fresnel theory, the continuous change of the effective refractive index between air and the underlying Si film is essential for suppressing light reflection. Thus the study is performed under the condition that the bottom diameter of SiSNF arrays is fixed to be square lattice period, i.e., $D_{bot} = \mathrm{P}$.

To understand the trend of absorption in the Si film based solar cells with SiSNF arrays, Fig. 2(a)–(c) display the absorption, reflection and transmission spectra of three representative structures, with different D_{bot} (200, 700, and 900 nm), both D_{top} and L are fixed to be 100 and 1000 nm, respectively. Note that the absorption spectra of the studied structure with D_{bot} (200 nm) owns Fabry–Perot-type resonances as that of the 2.33 μm thick Si film in the low energy region of 1.5–2.4 eV [22], while in the high energy the absorption is significantly enhanced. In addition, with increasing D_{bot}, the absorption edge significantly shifts toward the low energy region, which is attributed to irregularly cavity-resonances and guided mode resonances enhancement peaks [23].

For periodic structures, cavity-resonances and guided mode resonances enhancement peaks resonances stem from the coupling of incident light to a superposition of modes propagating in the plane of the arrays and strong Fabry–Perot resonances between the top and bottom interfaces [23]. In addition, the guided resonance peaks can only emerge at frequencies within the solar spectrum when the lattice constant (P) is sufficiently large [9]. As the number of guided modes increases with P, the irregularly mode resonances enhancement peaks analysis becomes increasingly complicated, however the same physical mechanisms still drive the absorption of SiSNF arrays. For $D_{bot} = 200$ nm, In the high energy region, antireflection of their front surface dominates the absorption enhancement behavior due to their stronger absorption coefficients and the graded refractive index between air and Si thin film. In the low energy range, high-order diffraction cut-off is the main reason of its lower absorption enhancement and the lower ultimate conversion efficiency. For $D_{bot} = 900$ nm, the absorption peaks degrade in the low energy region due to the high reflection loss and mode leakage. Higher ultimate efficiency is achieved in $D_{bot} = 700$ nm, due to the good antireflection performance, cavity-resonances and guide-resonances excitation in the absorption spectra over broadband and broad height range.

To quantitatively estimate the light trapping capability of the proposed structure over the solar spectrum, the ultimate efficiency (η) [24] is calculated from the following Eq. (1):

$$\eta = \frac{\int_{E_g}^{4.00} (E_g I(E) A(E)/E) dE}{\int_{0.31}^{4.00} I(E) dE} \tag{1}$$

where $E_g = 1.1$ eV is the band gap of crystalline silicon, E is photon energy, $I(E)$ is the solar energy density spectrum of ASTM (air mass 1.5 direct normal and circumsolar spectrum) [25], and $A(E)$ is the absorption spectrum. In this paper, the reason we focus on the solar spectrum (0.31–4 eV) for easy comparison with the previous report [7,9,20]. The upper limit of the integral is set as 4 eV, which is comparable to the upper limit of the spectrum of interest. The solar irradiance could be neglected when it is larger than 4 eV. The lower limit of the integral in the denominator is set as 0.31 eV, which is the lower limit of the available data for the solar spectrum. Provided that all the photons with the energy above E_g, which can be trapped by the proposed structure, could be converted into one electron–hole pair with the energy of E_g, and the electron–hole pair can be completely extracted for electrical energy output. The carrier recombination processes within the proposed structure are not taken into account. In other words, the internal quantum efficiency is assumed to be 100%.

Fig. 2(d) shows the ultimate efficiency as a function of D_{bot}. An ultimate efficiency (13.84%) for the 2.33 μm thick Si film based solar cells as the reference for easy comparison with the previous report [9]. Note that with increaseing D_{bot}, the ultimate efficiency peak appears at $D_{bot} = 700$ nm, which echo the variation of the absorption as shown in Fig. 2(a). Such phenomena can be explained that with further increasing D_{bot}, high reflection loss and mode leakage, which leads to energy loss. If this energy loss cannot be compensated by the absorption edge shift, the total light trapping capability would be degraded.

From the Fig. 2(d), the SiSNF arrays textured Si film based solar cells can achieve an ultimate efficiency of 31.60% when the parameters D_{top}, D_{bot}, H, and L take the values of 100, 700, 800, and 1000 nm, respectively. Such value is more than two times higher than that of 2.33 μm thick Si thin film based solar cells. In comparison, previous work showed that the Si nanopillar arrays textured Si film based solar cells with 800 nm thick underlying Si film and a periodicity constant of 500 nm can yield an ultimate efficiency of about 27% [7]. While the ultimate efficiency peak (30.54%) appears at $D_{bot} = 700$ nm for the silicon hexagonal nano-conical frustum (SiHNF) arrays surface texture based solar cells [20], and the ultimate efficiency of the SiSNF arrays is enhanced by 3.47% compared to SiHNF arrays. Accordingly, the $D_{bot} = 700$ nm is deemed as the optimized value and such structure is taken as the representative sample for the further studies.

Conventionally, the $4n^2$ enhancement is known as the Lambertian limit or the Yablonovitch limit. In this case, absoption (A) [26] is calculated in Eq. (2) as follows:

$$A = \frac{(1-e^{-2al})T}{1-e^{-2al} + (n_0^2/n_i^2)Te^{-2al}} \tag{2}$$

here l is the mean thickness of the sample, a is the optical absorption coefficient, n_i and n_0 are the refractive indices of the