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Light trapping in hybrid nanopyramid and nanohole structure silicon solar cell beyond the Lambertian limit

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We propose a hybrid nanostructure that comprises nanopyramids and nanoholes for thin film silicon (Si) solar cells. The hybrid structure demonstrates a stronger light trapping ability that is beyond the Lambertian limit. This is achieved with the smaller dimension nanohole structure which effectively reduces shorter wavelength light reflection, and the larger dimension nanopyramid structure which significantly enhances longer wavelength light trapping. An ultimate efficiency of 38.3% is yielded for a 2 μm thick Si cell incorporated with the hybrid structure, which is higher than that achievable corresponding to the Lambertian limit. Moreover, the high ultimate efficiency is retained as the incident angle increases from normal incidence to 50° for TM polarized sunlight. Therefore, the proposed hybrid structure is very promising to enhance the performance of thin film Si solar cells.

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I. INTRODUCTION

During the past decades, there has been intensive research and progress in photovoltaic as a viable renewable energy source. Silicon (Si) photovoltaic has dominated the global market due to its abundance, nontoxicity, and mature fabrication process.¹ However, a thick layer of Si over 200 μm is required to effectively absorb sunlight because of its low absorption coefficient. This has contributed significantly to the material cost and hence a key thrust of the research is on using thin film Si, instead of bulk Si, to lower the cost and yet without compromising the cell efficiency. To address the issue of weak optical absorption in Si thin films, nanostructures, such as nanowire,^{2,3} nanocone,⁴ and nanodome,⁵ have been incorporated for light trapping. Other techniques, such as plasmonic scattering⁶ and diffraction grating,⁷ have also been investigated. Although the above approaches have demonstrated a strong light trapping ability to boost light absorption, it still remains a challenge for the cell performance to reach the Lambertian limit, which sets the thermodynamic limit for light absorption.^{8–10} This limit is derived based on ray optic with incident light randomly scatters by a thin film.^{11–13} At this limit, the maximum optical path length is enhanced by $4n^2$ times, where n is the refractive index of the material. Such enhancement is important for long wavelength light near the band gap that has a small absorption coefficient.^{11–13}

Recent theoretical work has demonstrated the potential to reach the Lambertian limit based on wave optic.^{14–18} In this paper, we propose a hybrid nanostructure for thin film Si solar cells that combine nanopyramid (NP) and nanohole

(NH) structures, which exhibits efficiency that is higher than the Lambertian limit. The hybrid nanostructure is designed with the smaller NH to suppress light reflection for short wavelength light and the larger NP to enhance light trapping for long wavelength light. It is noted that the standalone NP and NH structures are not able to reach the Lambertian limit. However, by integrating them, a maximum ultimate efficiency (UE) of 38.3% at normal incidence has been achieved for a 2 μm thick Si solar cell with an optimized hybrid structure. This is higher than the Lambertian limit of 37.0% for the corresponding equivalent 1.33 μm thick Si thin film. The hybrid structure has also revealed a high UE at oblique incident angles up to 50° for TM polarized sunlight. Note that both the NP and NH structures can be fabricated by inexpensive approaches.^{10,19–21} Therefore, the proposed hybrid structure is promising in improving optical absorption and power conversion efficiency in thin film Si solar cells.

II. SIMULATION DETAILS

Figure 1 shows the (a) three-dimensional, (b) top, and (c) cross-sectional views of a thin film Si solar cell with the hybrid nanostructure. The nanostructure has a square unit cell of dimension P , which is also its period, and each cell comprises an inverted NP and a NH intersected at the apex of the NP. The height of the NP, which is from the base of the pyramid to the peak, is taken to be the same as the period P . The overall height of the hybrid structure is fixed at $T_1 = 1.5 \mu\text{m}$, while the overall thickness of the Si thin film is fixed at $T_2 = 2 \mu\text{m}$. On top of the hybrid structure is a thin layer of non-absorbing Si_3N_4 with a thickness t that serves as an antireflection and passivation layer. The hybrid structure is placed on a perfect electric conductor (PEC) at the bottom,

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FIG. 1. The simulated hybrid structure of nanopyramid and nanohole thin film solar cell structure. (a) Three-dimensional schematic, (b) top view, and (c) cross-sectional view of the hybrid structure. The blue color represents Si material, while the yellow color refers the nonabsorbing Si_3N_4 that is on top of the hybrid structure. The red color represents the perfect electric conductor.

which serves a similar function as the metal electrode in a real device to reflect sunlight back to the hybrid structure. The optical constants of the crystalline Si and Si_3N_4 are taken from the literature.²² A full wave finite element method (FEM) was used to simulate the interaction between the incident light and the solar cell.²³ By solving the Maxwell's equation, the spatial electric field distribution in the solar cell can be obtained, from which its optical characteristics can be calculated. To optimize the cell performance, the structure periodicity P was varied from 400 nm to 1000 nm, the diameter to period (D/P) ratio of the NH from 0.3 to 0.9, and the thickness of Si_3N_4 t from 20 nm to 100 nm. The incident light has a wavelength (λ) range from 300 nm to 1130 nm, covering the main solar spectrum of interest for Si. For comparison of photovoltaic performance of cells with different structural parameters, the UE was calculated by assuming perfect internal quantum efficiency.^{9,24}

III. RESULTS AND DISCUSSION

We have studied light absorption of the hybrid nanopyramid and nanohole structure at different P from 400 to 1000 nm, in step of 100 nm, and at a fixed D/P ratio of 0.7. Figure 2 shows the results at three selected P of 400 nm, 800 nm, and 1000 nm. It is found that due to the introduction of the hybrid nanostructures, the light absorption is generally high and above 80% for $\lambda < 600$ nm. When P is small at 400 nm, the light absorption for $\lambda > 600$ nm is relatively low as the periodicity is much smaller than the wavelength, and there is no strong scattering of light induced. For larger P of 800 nm, the light absorption is substantially increased for

FIG. 2. Light absorption spectra of the hybrid structure at different P and a fixed D/P ratio of 0.7.

longer and comparable wavelength over the range of $\lambda > 600$ nm. When P is further increased to 1000 nm, there is a drop in absorption for $600 \text{ nm} < \lambda < 1000$ nm, but an increase for $\lambda > 1000$ nm that is above the Lambertian limit. Overall, the optimum structural periodicity is found to be 800 nm.

We have also studied the light absorption of the hybrid nanopyramid and nanohole structure at the optimum P of 800 nm and different D/P ratios from 0.3 to 0.9, in step of 0.1. The results at three selected D/P ratios of 0.3, 0.7, and 0.9 are shown in Fig. 3. At the small D/P ratio of 0.3, the diameter of the nanohole structure is small and strong scattering is induced for shorter wavelength light due to its comparable wavelength with the dimension of the nanostructure. Indeed, the light absorption is approaching 100% over the range of $300 \text{ nm} < \lambda < 600$ nm. When the D/P ratio increases to 0.7, the light absorption is weakened for shorter wavelength light with $\lambda < 500$ nm, but increases for longer wavelength light. As the D/P ratio is further increased to 0.9, the light absorption is overall diminished over the longer wavelength range of $\lambda > 600$ nm. This is because at large D , there will only be little Si material available for absorption. Overall, the optimum D/P ratio is found to be 0.7.

FIG. 3. Light absorption spectra of the hybrid structure at the optimum P of 800 nm and different D/P ratios.

Therefore, the optimized hybrid structure that gives rise to the highest UE has the following structural parameters, $P = 800$ nm, $D = 560$ nm, and $t = 80$ nm. Note that the UE is calculated by assuming an internal quantum efficiency of 100% and it defines the theoretical limit for the maximum power conversion efficiency that can be achieved for the solar cell.²⁵ In such a calculation, the focus is essentially on the optical absorption of the hybrid structure while assuming a perfect transport and collection of the photogenerated carriers. The ultimate efficiency is determined by the energy band gap and the complex refractive index of Si. Its dependence on the Si doping is very weak as it is mainly through the effect of the doping on the complex refractive index. In Fig. 4, we compare light absorption of the optimized hybrid structure, the planar film without nanostructure, and the Lambertian limit of the corresponding equivalent $1.33 \mu\text{m}$ thick Si thin film. The Si planar film has the same thickness of $2 \mu\text{m}$ as the hybrid structure, and with an 80 nm thick Si_3N_4 layer on top and a PEC layer at the bottom. It is clearly seen that light absorption in the hybrid structure is high over a broadband and is significantly enhanced compared with the planar film. For shorter wavelength of $\lambda < 450$ nm, the absorption is around 90% and slightly lower than that of the Lambertian limit which is approaching 100%. For $450 \text{ nm} < \lambda < 700$ nm, which covers the main solar spectrum, the absorption of the hybrid structure is 95%, which is much better than that of the planar film and is comparable with the Lambertian limit. For $700 \text{ nm} < \lambda < 800$ nm, the absorption in the hybrid structure is slightly lower than the Lambertian limit. However, for $800 \text{ nm} < \lambda < 1100$ nm, it is generally higher than the Lambertian limit, indicating the strong light trapping ability of the hybrid structure at long wavelength. Compared with the planar film without the nanostructure, the hybrid structure demonstrated much improved light absorption enhancement over the whole solar spectrum. For the short wavelength light region, the light absorption enhancement is mainly contributed by the smaller nanohole structure. For the longer wavelength light, the enhancement is due to the larger pyramid structure. The optimized hybrid

FIG. 4. Absorption spectra of the optimized hybrid structure, planar Si thin film cell of $2 \mu\text{m}$ thick, and Lambertian limit absorption for $1.33 \mu\text{m}$ thick Si thin film cell.

structure has a high UE of 38.3%, as compared with the Lambertian limit of 37.0%. Hence, it offers a potential means to surpass the Lambertian limit and achieve high efficiency thin film Si solar cells.

In order to achieve a high broadband light absorption and hence high efficiency solar cell, it is critical to suppress light reflection at shorter λ and improve light trapping at longer λ . For shorter $\lambda < 700$ nm, the design consideration is focused on suppressing light reflection at the top surface. Firstly, due to the gradual change in the size of the NP, light scatters and couples effectively into the hybrid structure owing to much improved refractive index matching.^{26,27} In addition, the comparable feature size of the NH with the shorter λ and the antireflection coating have played a role in achieving this objective. For longer $\lambda > 700$ nm, the focus is on improving light absorption since the absorption coefficient is weak in Si in this wavelength range. When P is much smaller than λ , only a few guided resonance modes are excited in the Si thin film and hence light absorption enhancement is marginal. On the other hand, when P is much larger than λ , although more guided resonance modes are excited, they are easily coupled and leaked to the increased external channels.^{14,18,28} When P is comparable but slight smaller than λ , the number of guided resonance modes increases quadratically with decreasing λ ,^{14,18} and the maximum absorption is achieved when $P = \lambda$, giving rise to an enhancement factor of $4\pi n^2$.^{14,18} Therefore, at $P = 800$ nm, the NP and NH can effectively guide the incident light within the hybrid structure, resulting in enhanced absorption above the Lambertian limit for $800 \text{ nm} < \lambda < 1100$ nm. There was a slight drop in absorption when $\lambda < P$ is attributed to an increase in the number of leakage channels. Hence light is not well confined in the hybrid structure, but is instead leaked through higher order channels.^{14,18} Overall, the optimized hybrid structure has achieved a much improved light absorption by suppressing light reflection with the smaller feature size NH structure and enhancing light trapping due to the excited guided resonances from the larger size NP.

Figure 5 shows the angular dependence of the UE of the hybrid structure for both TE and TM polarized lights. The

FIG. 5. The angular dependence of the ultimate efficiency of the hybrid cell for both TE and TM polarized light.

UE is nearly constant for both polarizations of light when the incident angle (θ) is less than 10° . Beyond that, it decreases with the rate being faster for the TE polarized light. Note that the UE is still larger than the Lambertian limit up to $\theta = 50^\circ$ for TM polarized light, and it is maintained above 34% even at $\theta = 70^\circ$. The decrease in light absorption at larger θ is attributed to an increase in coupling to the leakage channels at increasing θ , resulting in a substantial reduction in light absorption.¹⁴ It is worth noting that the high UE observed even at larger θ suggests that the hybrid structure is very promising for practical application as sunlight is rarely incident normally on solar cell.

We have also studied the effect of varying the nanopyramid height on the absorption of the hybrid structure. It is noticed that there is only a slight variation of 1–2% in the ultimate efficiency when the height of the nanopyramid is varied over the range from 400 to 1200 nm. However, it is expected that if the nanopyramid height is substantially reduced below 400 nm or increased close to the overall hybrid structure height of $1.5\ \mu\text{m}$, the ultimate efficiency will fall as the hybrid structure will then revert to the standalone nanopyramid or nanohole structure, both of which are not as efficient as the hybrid structure in light absorption.

IV. CONCLUSIONS

In summary, we have proposed a hybrid solar cell structure that comprises nanopylramids and nanoholes. The optimized structure has a periodicity of 800 nm, nanohole diameter of 560 nm, and Si_3N_4 thickness of 80 nm. The hybrid solar cell has light absorption that is substantially increased above the Lambertian limit, achieving an ultimate efficiency of 38.3%. The UE is maintained above the Lambertian limit even for incident angle up to 50° for TM polarized sunlight. The results suggest that the proposed hybrid nanostructure is very promising in achieving high efficiency thin film Si solar cells.

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