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Citation: Journal of Applied Physics 114, 024305 (2013); doi: 10.1063/1.4813096

View online: http://dx.doi.org/10.1063/1.4813096

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Optimal design of nano-scale surface light trapping structures for enhancing light absorption in thin film photovoltaics

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(Received 5 April 2013; accepted 18 June 2013; published online 11 July 2013)

We present the effect of nanophotonic light trapping structures on optical absorption enhancement of crystalline silicon thin film solar cells, based on a rigorous coupled-wave analysis method. The calculation involves three different structures (i.e., hole, inverted-cone, and inverted-paraboloid), which are commonly applied on the top surface of thin film solar cells. Systematical calculation results in terms of geometrical parameters reveal sweet spots (i.e., optimum geometric structure) to obtain the highest cell efficiency for each structure, which provide a design guideline in thin film photovoltaic devices. © 2013 AIP Publishing LLC. [http://dx.doi.org/10.1063/1.4813096]

I. INTRODUCTION

Thin film photovoltaic (PV) techniques have attracted considerable interest due to their potential to reduce the cost of solar electricity by reducing the amount of photoactive materials. However, the poor light absorption feature near the band gap edge of the photoactive material and the thin absorption layer limit the efficiency of thin film PV cells.^{1,2} Hence, efficient light management is inevitably necessary to improve efficiency in thin film PV cells. Over recent years, several approaches have been explored to manage incident light efficiently in thin films with light trapping structures and plasmonic structures.²⁻⁴ Two dimensional rod or hole arrays with nano-scale periods are commonly used structures for light trapping. Recently, theoretical studies and experimental demonstrations have been executed to improve light absorption with these rod/hole structures on the solar cells. 5-9 Together with advanced fabrication techniques, nanostructures with a tapered profile were also developed and applied to various optical devices, including light emitting diodes, photodetectors, solar cells, and transparent glasses/polymers. 10-13 These inclined structures, which are called "moth eye" structures, can reduce the unwanted surface reflection over broad wavelength ranges when the period of the structures is smaller than the optical wavelength. Although various structures have been developed for increasing the cell efficiency in thin film solar cells, there are relatively few studies on global design comparisons between various geometries for maximizing the cell efficiency.

In this paper, we systematically investigated the absorption characteristics of crystalline silicon (c-Si) thin film with three important light trapping structures, i.e., hole, inverted-cone, and inverted-paraboloid arrays, which are structures that can be generated by existing nano-technologies. ^{9,13,14} The geometrical parameters were optimized to achieve high efficiency c-Si thin film solar cells via a rigorous coupled-wave analysis

method. The effective absorption capability of the c-Si thin

II. STRUCTURES AND SIMULATION METHOLOGY

Figures 1(a)–1(c) illustrates the schematic of the c-Si thin film with hole, inverted-cone, and inverted-paraboloid arrays, respectively. Figure 1(d) shows the top view of a square lattice area with a side length equal to a period. An aluminium (Al) metal back reflector is incorporated onto the bottom side for light trapping enhancement. In this study, the thickness of c-Si film and Al back reflector was fixed as $2 \mu m$ and 30 nm, respectively. The wavelength range of the normally incident light onto the surface varies in the range 310–1127 nm (4 to 1.1 eV), which covers the major solar energy spectrum that is of interest in c-Si based solar cells. Figure 1(e) shows the change of the calculated effective refractive index, which is determined using the volume weighted average refractive index of air $(n_{air} = 1)$ and c-Si $(n_{c-Si} \sim 3.8)$, of the structures corresponding to the depth. The large refractive index difference between air and c-Si at the top surface causes a significant increase in Fresnel reflection. To overcome this problem, the refractive index difference was reduced by setting the surface diameter identical to the period (i.e., a diameter-to-period ratio of 1). The effective refractive index of the hole structure abruptly changes from ~ 1.6 to ~ 3.8 , while the effective refractive index of the inverted-cone and inverted-paraboloid structures gradually change from ~ 1.6 to ~ 3.8 . In particular, the inverted-paraboloid structure exhibits an almost linearly graded index profile, which is the most appropriate index profile to reduce the Fresnel reflection. 15,16

III. RESULTS AND DISCUSSION

To achieve high efficiency in c-Si thin film solar cells, the period of surface light trapping structure, which strongly

films considering the intensive solar energy spectrum was quantitatively estimated by calculating the ultimate efficiency (η_u) . The cell efficiency was also calculated to estimate the efficiency of c-Si thin film solar cells with various nano-scale surface light trapping structures.

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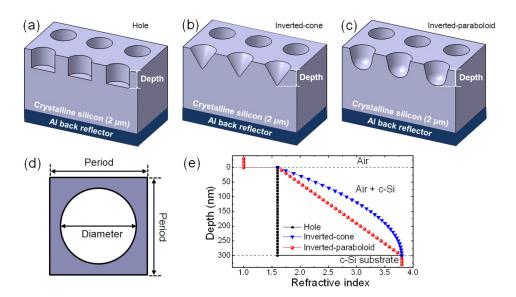


FIG. 1. Schematics of the c-Si thin film with nano-scale (a) hole, (b) inverted-cone, and (c) inverted-paraboloid arrays. (d) The top view of a square lattice area. (e) The calculated effective refractive index of the structures used in the simulation corresponding to the depth. The maximum depth is fixed at 300 nm and the diameter is identical to the period.

influence the absorption characteristics of c-Si thin film, ⁴⁻⁷ was first considered. Figures 2(a)–2(c) show the contour plots of absorption spectra of the c-Si thin films for the period variation of the hole, inverted-cone, and inverted-paraboloid structures, while fixing the depth and diameter-to-period ratio as 300 nm and 1, respectively. In the contour plots, ripple patterns appear due to the interference of the reflected light from the top surface and the c-Si/Al interface. The absorption increases as the period decreases in the short wavelength regimes. This can be attributed to the comparable period of the structures with the incident light into the

c-Si because the incident light can easily penetrate the objects without considerable interruption, when the dimensions are smaller than the wavelength of incident light. ^{4,16} It is found that the absorption regions exceeding 30% broaden toward the long wavelength regions as the period increases mainly due to the shift of reflection minima toward the long wavelength regions. ^{4,16} It should be pointed out that the density of solar energy is not uniform within the solar spectrum; ¹⁷ therefore, it is important to find the optimum period of the surface light trapping structures for maximizing the light absorption by considering the solar spectrum. Hence,

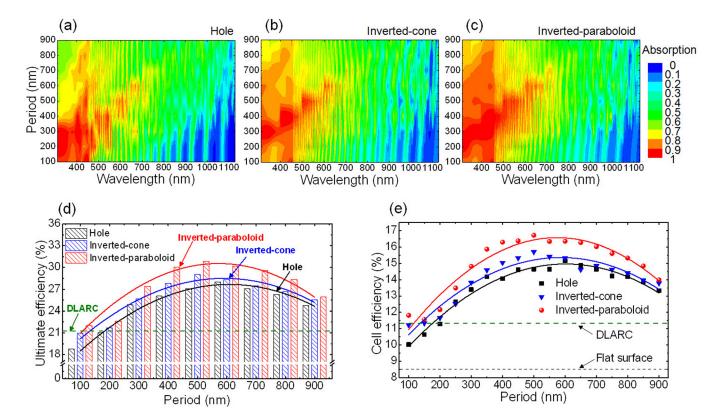


FIG. 2. Contour plots of the absorption spectra of the c-Si thin films for the period variation of the (a) hole, (b) inverted-cone, and (c) inverted-paraboloid structure as a function of wavelength. The calculated (d) ultimate efficiency and (e) cell efficiency of the c-Si thin films with three different light trapping structures for the period variation. The depth was fixed at 300 nm and the diameter-to-period ratio was 1.

we calculated the η_u according to the period of the light trapping structures in order to quantitatively estimate the light absorption capability of the structures at the terrestrial air mass 1.5 global (AM 1.5 G) by using the formula 6,18,19

$$\eta_{u} = \frac{\int_{10 \text{ nm}}^{\lambda_{g}} I(\lambda) \alpha(\lambda) \frac{\lambda}{\lambda_{g}} d\lambda}{\int_{310 \text{ nm}}^{4000 \text{ nm}} I(\lambda) d\lambda},$$
(1)

where $I(\lambda)$ is the spectral energy density at the AM 1.5 G, $\alpha(\lambda)$ is the absorption, and λ_g is the wavelength corresponding to the band gap of c-Si. In Eq. (1), the upper limit of 4000 nm corresponds to the upper limit of the available data for the solar spectrum. To calculate the η_u , it is assumed that each photon with energy greater than the band gap would be absorbed and would generate one electron-hole pair with energy identical to the band gap energy, and that all carriers are completely extracted for electrical energy output. 19 That means that the recombination processes of the generated electron-hole pair are not considered. It is also worth noting that the excess energy of the absorbed photons above the band gap is dissipated; thus the contribution of the absorbed solar energy to η_u decreases as the photon energy increases from the band gap. Figure 2(d) shows the period dependent the η_u for the light trapping structures. The calculated η_u of a c-Si thin film with double layer antireflection coating (DLARC) composed of 80 nm-thick SiN_x and 84 nm-thick SiO₂, 21.20%, is shown as a reference. It is observed that the η_u first increase with an increasing period and then begins to decrease as the period further increases. This behavior of η_u corresponding to the period increase can be predominantly attributed to the shift of high absorption regions from a weak energy density region (short wavelength region) to a relatively high energy density region (long wavelength region), going through the main energy density region (around 500 nm) of the solar energy spectrum with an increasing period, 4,16,18 as can be seen in Figures 2(a)-2(c). The maximum η_u of the c-Si thin films with the light trapping structures are much higher than the η_u of the c-Si with a flat surface (15.97%) and DLARC. The c-Si thin film with the inverted-paraboloid light trapping structure demonstrates the highest η_u of 30.86% at the period of 500 nm.

We also calculated cell efficiency to estimate the influence of the geometric parameters of the light trapping structures on the efficiency of c-Si thin film solar cells by the equation $\eta = J_{sc}V_{oc}\Gamma_f/P_{in}$, where J_{sc} is the short-circuit current density, V_{oc} is the open-circuit voltage, Γ_f is the fill factor, and P_{in} is the incident solar power under AM 1.5G. The relationship between J_{sc} and η_u is given by 18,20,21

$$J_{sc} = \eta_c \int_{310 \text{ nm}}^{\lambda_g} I(\lambda) \alpha(\lambda) \frac{e\lambda}{hc} d\lambda = \eta_c \eta_u \frac{e\lambda_g}{hc} \times \int_{310 \text{ nm}}^{4000 \text{ nm}} I(\lambda) d\lambda$$
$$= 81.83 \eta_c \eta_u (\text{mA/cm}^2), \tag{2}$$

where η_c is carrier collection efficiency, e is the electron charge, h is Plank's constant, and c is the speed of light. V_{oc} was obtained from $V_{oc} = (kT/e) \ln(J_{sc}/J_{s0} + 1)$ (in volts), where k is the Boltzmann's constant, $T = 300 \,\mathrm{K}$, and J_{s0} is the reverse bias saturation current. In our calculation, a η_c of 85% with a 5% shadowing effect from electrodes was taken into account. The J_{s0} was taken to be 1.5×10^{-15} A/cm², and a fill factor of 80% was used. The details of the efficiency calculation can be found in the literature.²¹ Figure 2(e) shows the calculated cell efficiency for the three different light trapping structures as a function of the period. The calculated cell efficiency of the thin film c-Si with a flat surface (8.50%) and DLARC (11.37%) are shown as a reference. The calculated cell efficiencies of the c-Si thin films with the light trapping structures exhibit higher cell efficiency than the one with a flat surface and have the same behavior as the η_u because the cell efficiency depends on the light absorption. The maximum cell efficiencies of the c-Si thin films with hole, invertedcone, and inverted-paraboloid structure were 15.15%, 15.71%, and 16.72%, respectively, corresponding to a period of 600 nm for the hole and a period of 500 nm for the inverted structures. This indicates that the maximum cell efficiency of solar cells with light trapping structures relies on the shape and period of light trapping structures. Thus, it is crucial to employ a light trapping structure with an optimum shape and period for achieving high efficiency solar cell.

The depth of surface light trapping structures is an important geometric parameter to achieve high efficiency c-Si thin film solar cells because the effective refractive index of the tapered structure is more gradually graded, which results in more suppression of the Fresnel reflection, as the depth of the tapered part increases.^{4,15,16} Figure 3(a) shows variation of the calculated cell efficiencies for the light trapping structures depending on the depth, while fixing the period of the hole and inverted light trapping structures as 600 nm and 500 nm, respectively. In this simulation, the diameter-to-period ratio of the structures was set at 1. The cell efficiencies of the c-Si thin films with the inverted structures gradually increase at the initial stage due to the suppression of reflection, but they are saturated due to the reduction of the absorber volume with the increasing depth. The hole structure exhibits a somewhat different behavior compared to the inverted structures. The hole structure acts as an effective medium that approximates a single layer thin film. Thus, the optical property of the hole structure is similar to that of a single layer antireflection coating. 12 For this reason, the cell efficiency of the c-Si thin film with hole structures is maximized when the depth of the hole is 300 nm (15.15%), and then decreased mainly owing to the reduction of the absorber volume. Among the light trapping structures we used, the inverted-paraboloid structure again demonstrates the highest cell efficiency of 17.18% at a depth of 500 nm, which is more than double the cell efficiency for the c-Si thin film with a flat surface. This result means that the depth of surface light trapping structures is also an important parameter for maximizing the efficiency of solar cells.

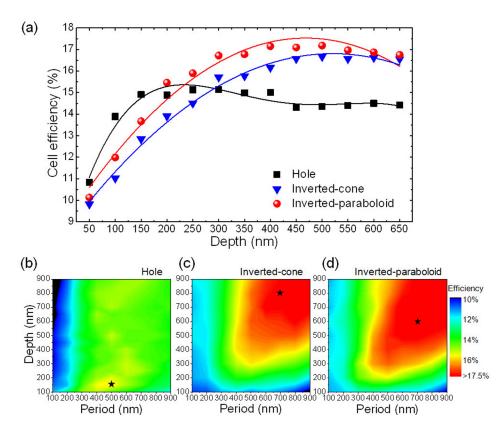


FIG. 3. (a) The calculated cell efficiencies for the light trapping structures as a function of the depth corresponding to a period of 600 nm for the hole structure and a period of 500 nm for the inverted structures. (b) Contour plots of the calculated cell efficiencies for the light trapping structures as a function of the period and depth. The diameter-to-period ratio was fixed as 1.

In order to find the optimum period and depth of each surface light trapping structure, multi-parameter scan, which has not been yet performed in the previous studies, 5-7 was carried out for various periods and depths. Figures 3(b)-3(d)shows contour plots of the cell efficiencies for the c-Si thin films with the hole, inverted-cone, and inverted-paraboloid structures as a function of the period and depth. The cell efficiency strongly correlates with both the period and depth of the surface light trapping structures. The inverted structures show higher cell efficiency than the hole structure except in the low depth regions. The inverted-paraboloid structure shows relatively higher cell efficiency than the inverted-cone structure. The maximum cell efficiencies of the c-Si thin films with hole, inverted-cone, and inverted-paraboloid structure were 15.64%, 17.74%, and 18.02%, respectively, corresponding to a period of 500 nm and a depth of 150 nm for the hole, a period of 700 nm and a depth of 800 nm for the inverted-cone structure, and a period of 700 nm and a depth of 600 nm for the inverted-paraboloid structure. In addition, we investigated the influence of cell thickness on both the optimum period and depth of the surface light trapping structures by increasing the cell thickness (5 μ m and $8 \mu m$). For the hole structure, the optimum depth was not changed; however, the optimum period was slightly reduced. The optimum periods and depths of the inverted structures were increased compared to the optimum values for the $2 \mu \text{m}$ -thick c-Si solar cells. The maximum cell efficiencies of the c-Si solar cells with surface light trapping structures and a flat surface were increased with increasing cell thickness due to enhanced light absorption, particularly in the long wavelength regions. It is noteworthy that the invertedparaboloid structure showed the highest maximum cell efficiency for a given cell thickness. The optimum periods, depths, and maximum cell efficiencies corresponding to the cell thickness are summarized in Table I.

So far, we have assumed that the diameter-to-period ratio is 1 in order to minimize the degree of discontinuity in the effective refractive index of c-Si thin films at the top surface (i.e., minimize Fresnel reflection at the surface). From the viewpoint of practicality, however, diameter-to-period ratio close to 1 imposes a burden on the fabrication procedure. Hence, it is necessary to investigate the influence of the diameter-to-period variation on cell efficiency. Figure 4(a) shows the calculated cell efficiencies for the light trapping structures with the optimum period and depth on $2 \mu m$ -thick c-Si thin film as a function of the diameter-to-period ratio. As the diameter-to-period ratio becomes close to 1 (i.e., by reducing the mismatch of effective refractive index between air and c-Si at the surface), the cell efficiency for the inverted structures progressively increases due to a more gradually graded effective refractive index, which results in a better

TABLE I. Optimum periods, depths, and maximum cell efficiencies for the hole, inverted-cone, and inverted-paraboloid light trapping structures corresponding to the thickness of c-Si solar cell.

	Hole			Inverted-cone			Inverted-paraboloid		
Thickness (µm)	2	5	8	2	5	8	2	5	8
Period (nm)	500	400	400	700	900	900	700	900	800
Depth (nm)	150	150	150	800	1100	1100	600	800	1100
Efficiency (%)	15.64	20.14	22.38	17.74	22.37	23.67	18.02	22.44	24.17

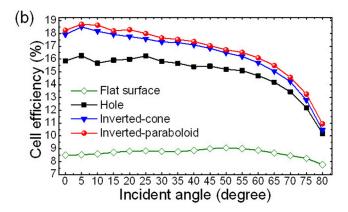


FIG. 4. (a) The calculated cell efficiencies of the c-Si thin films with three different light trapping structures with the optimum period and depth for the diameter-to-period ratio variation. (b) The calculated cell efficiencies for the optimized surface light trapping structures and a flat surface as a function of the incident angle of light.

suppression of Fresnel reflection. Interestingly, the slope of efficiency increase for the hole structure is decreased as the diameter-to-period ratio comes close to 1. This may be attributed to compensation between the light trapping improvement inside the hole structure and the fast reduction of the absorber volume as the diameter increases. From these results, we can find that the optimum geometric parameters for the hole structure (a period of 500 nm, a depth of 150 nm, and a diameter of 500 nm), inverted-cone structure (a period of 700 nm, a depth of 800 nm, and a diameter of 700 nm), and inverted-paraboloid structure (a period of 700 nm, a depth of 600 nm, and a diameter of 700 nm) to achieve the highest cell efficiency. Although the optimum hole structure and inverted structures are difficult to precisely realize on a 2 µm-thick thin film c-Si with a metal back reflector, the metal-assisted chemical etching method,⁹ and the dry etching of etch mask with inverted profile formed by various nanopattering techniques^{13,14} are potential approaches. It is predicted that the increased surface area by introducing the light trapping structures on the surface of solar cells causes surface recombination losses which degrades the electrical properties of the solar cell. Thus, the surface passivation layer is necessary to prevent the performance degradation of solar cells due to surface texturing for practical applications.²²

The incident angle-dependent light trapping characteristics of the light trapping structures are considerably important to achieve high and stable solar cell efficiency during the day. Thus, we investigated the cell efficiency of the c-Si

thin films with the optimized hole, inverted-cone, and inverted-paraboloid structure for the oblique light incidence. Figure 4(b) shows the calculated cell efficiencies for the three different light trapping structures on 2 µm-thick c-Si thin film as a function of the incident angle of light. The incident angle-dependent cell efficiency for a flat surface is shown as a reference. As the incident angle increases, the cell efficiency of the c-Si thin films with light trapping structures decreases due to increased surface reflection loss. At a slightly oblique incident angle, interestingly, the cell efficiency is enhanced due to the prolonged optical path length of light by tilting the incident light.²¹ All light trapping structures exhibit much higher cell efficiency than the flat surface in an incident angle range of 0°-80°. Among the optimized light trapping structures, the inverted-paraboloid structure consistently demonstrates the highest cell efficiency over the entire incident angle of light. The nano-scale inverted light trapping surface structures with a tapered profile have a great potential for achieving high and stable efficiency thin film PV cells.

IV. CONCLUSIONS

We investigated the absorption characteristics of c-Si thin films with hole, inverted-cone, and inverted-paraboloid light trapping surface structures and optimized their geometric parameters to achieve high cell efficiency. It was found that the geometric parameters, including shape, period, depth, and diameter-to-period ratio, of the light trapping structures as well as the cell thickness affect the efficiency of thin film PV cells. We found that the inverted-paraboloid structure exhibited the highest cell efficiency and incident angle-dependent cell efficiency among the optimized light trapping structures. These results provide a guideline for the optimum design of thin film PV cells with surface light trapping structures.

ACKNOWLEDGMENTS

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MEST) (No. 2011-0017606).

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