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Simulated optical absorption enhancement in random silicon nanohole structure for solar cell application

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We have conducted a systematic simulation study on light absorption in a silicon nanohole structure that has randomness introduced into its structural parameters, which include the hole radius, depth, and position. It is found that light absorption is enhanced for the random structures compared to their periodic counterparts. This is attributed to additional resonances induced by the structural disorders, broadening of the existing resonance, and lower optical reflection. The highest light absorption is obtained for the structure with randomness in hole position, which achieves a 12.7% enhancement compared with the periodic structure. © 2014 AIP Publishing LLC.
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I. INTRODUCTION

Due to the high cost and environmental issues associated with the use of traditional fossil fuel, alternative renewable energy sources such as photovoltaic have been extensively explored. Among the various types of solar cells, silicon (Si) solar cells are the most established and have dominated the market due to its abundance, nontoxicity, and mature fabrication process.[1] However, bulk Si solar cell requires a few hundred micrometers thick of Si to effectively absorb sunlight, which contributes substantially to its cost and impedes its widespread application. To render Si solar cells more cost competitive, Si nanostructures, such as nanowire,[2,3] nanodome,[4] and nanocone,[5] have been introduced for light trapping so that the thickness of Si layer needed is reduced. So far, most of the experimental and theoretical works in this area focus on periodic nanostructures, which are technologically challenging to achieve and costly to realize over a large area. There exist simple and low cost techniques to fabricate nanostructures,[6,7] which nevertheless give rise to disorders such as variations in the positions and dimensions of the nanostructures. To date, the effects of such disorders on the optical performance of the nanostructures have not been extensively studied. Recently, Bao *et al.*,[8] Du *et al.*,[9] and Lin *et al.*[10] have investigated theoretically light absorption for a nanowire structure with random wire length, diameter, and position. In addition, Lin has also investigated the nanohole structure.[11] It was found that light absorption is improved due to the presence of additional resonance modes and broadening of the existing modes. We have previously studied silicon nanohole (SiNH) structure, which has been found to be better than SiNW structure in terms of improved light absorption, carriers transport, and mechanical robustness.[7,12,13] In this paper, we further investigate the optical characteristics of SiNH with randomness introduced into its

structural parameters, which include the nanohole radius, depth, and position. The results are compared with periodic SiNH structures, and it is found that the random structures offer substantially improved light absorption. The highest absorption is achieved for the structure with random hole position. An ultimate efficiency of 33.8% is obtained, which is 12.7% higher than that of a periodic structure.

II. SIMULATION METHODOLOGY

Figure 1(a) shows the schematic of the periodic nanohole structure (PNS), while Figs. 1(b), 1(c), and 1(d) show the random nanohole structures (RNS) with, respectively, randomness in the radius (R), depth (D), and position of the holes. For the PNS, D is fixed at 1 μm and there is an
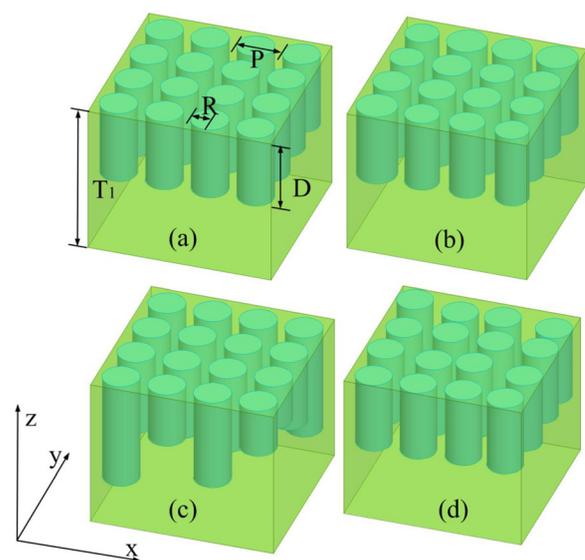

FIG. 1. Schematic illustration of (a) periodic SiNH structure, and random SiNH structures with variation in (b) hole radius, (c) hole depth, and (d) hole position.
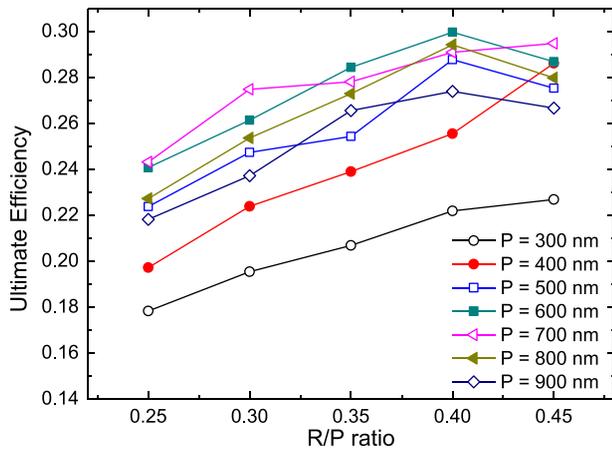
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FIG. 2. Ultimate efficiency of the periodic nanohole structure with varying structural periodicity P as a function of the radius/periodicity (R/P) ratio.

underlying Si film of 1 μm thick, such that the total thickness of Si is $T_1 = 2 \mu$m. We have simulated the effects of the structural parameters on the optical absorption of the PNS, and identified the optimum structure with R = 240 nm and periodicity P = 600 nm, that gives rise to the highest ultimate

efficiency of 30.0%. This is illustrated in Fig. 2 that plots the ultimate efficiency of the PNS as a function of its hole radius and periodicity, at a fixed hole depth of 1.0 μm. In terms of optimum hole depth, we have simulated PNS with hole depth D of 0.5 μm, 1.0 μm, and 1.5 μm, and with the hole periodicity and radius fixed at their optimum values. The corresponding simulated ultimate efficiencies are 29.3%, 30.0%, and 28.2%. It is seen that the ultimate efficiency is not sensitive to the depth of the SiNH over the range studied and hence we have chosen a hole depth of 1 μm for the optimum PNS, which gives rise to the best ultimate efficiency of 30.0%. The slight decrease in the ultimate efficiency observed at D = 1.5 μm is attributed to the structure having less Si material for absorption. Note that for all the 3 PNS with different depths, their ultimate efficiencies are much better than the 13.9% obtained for planar Si thin film without SiNHs. The optimum periodic structure will serve as a starting point and reference for our simulation studies to introduce randomness into the structure. For the simulation of RNS, we define a square unit cell with an area of 2.4 μm by 2.4 μm on the x-y plane. Each unit cell is divided into 16 smaller 600 nm by 600 nm sub-cells, with each sub-cell having a SiNH centered within it. This corresponds to the optimum periodicity
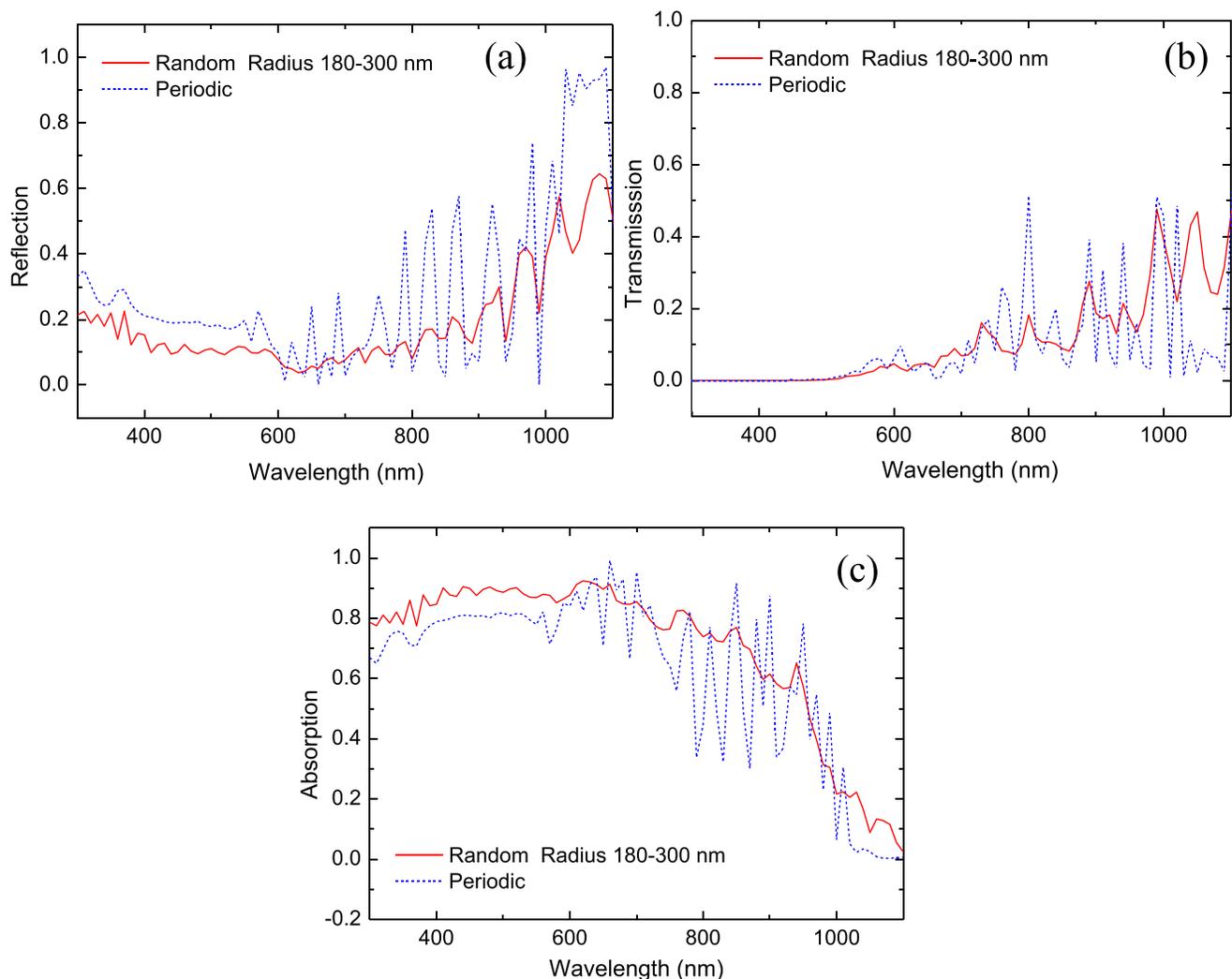

FIG. 3. (a) Light reflection, (b) transmission, and (c) absorption of the SiNH structure with random hole radius.

deduced of P = 600 nm. The 16 SiNHs in the sub-cells have either their depths, positions, or radii randomly generated within certain ranges, as shall be explained shortly. For the 2.4 μm by 2.4 μm unit cell, a perfectly matched layer boundary condition is applied in both the $\pm$z directions, while periodic boundary condition is used in both the x and y directions to simulate a large area two dimensional structure.

For the RNS with random hole depth, D is allowed to vary randomly from its original value of 1 μm by $\pm$20%, that is, D varies from 0.8 μm to 1.2 μm, while R is fixed at its optimum value. This variation is based on our experimental observation of SiNH fabricated using the electroless chemical etching with Ag catalyst formed by laser annealing of a thin Ag film.[7,12] For the fabricated non-periodic SiNH structure, the radius is correlated to the thickness of the starting Ag layer, and generally is not well-controlled and varies over a wide range. For our simulation of RNS with random radius, R is allowed to vary randomly from its optimum value of 240 nm by $\pm$ 60 nm, reaching the maximum possible radius without overlapping with neighboring holes in adjacent sub-cells, while D is fixed at its optimum value. Note that the case of R = 300 nm corresponds to the situation where each SiNH occupies the entire sub-cell. Similarly, for the RNS with random hole position, each hole is allowed to change its original center position within one sub-cell by a

maximum of $\pm$60 nm in both x and y directions, while R and D are fixed at their optimum values. The case of the hole position shifted by 60 nm would correspond to the SiNH located at the edge of the sub-cell. We further illustrate the simulation process using the case of random radius structure as an example. We first used Matlab to randomly generate 16 uniformly distributed nanohole radii, which are then fed into the simulation software to simulate the optical absorption of the random radius structure. To ensure that the optical characteristics simulated truly reflect randomness in the nanohole radius, the process is repeated eight times to generate eight different sets of uniformly distributed random radii, and to simulate their corresponding absorption spectra. The final absorption spectra presented is an average of all the eight absorption spectra. Note that our approach does not reflect a truly random structure, but instead a quasi-random structure to help understand the effect of non-periodicity on the absorption characteristics of the structures. To simulate a truly random structure would not be possible due to the tremendous computing resources required for the case of a full-wave simulation. Nevertheless, the averaging of the absorption spectra will help ensure that the optical characteristics simulated are close to a truly random structure.

The optical characteristics of these nanohole structures were simulated using the commercial software High
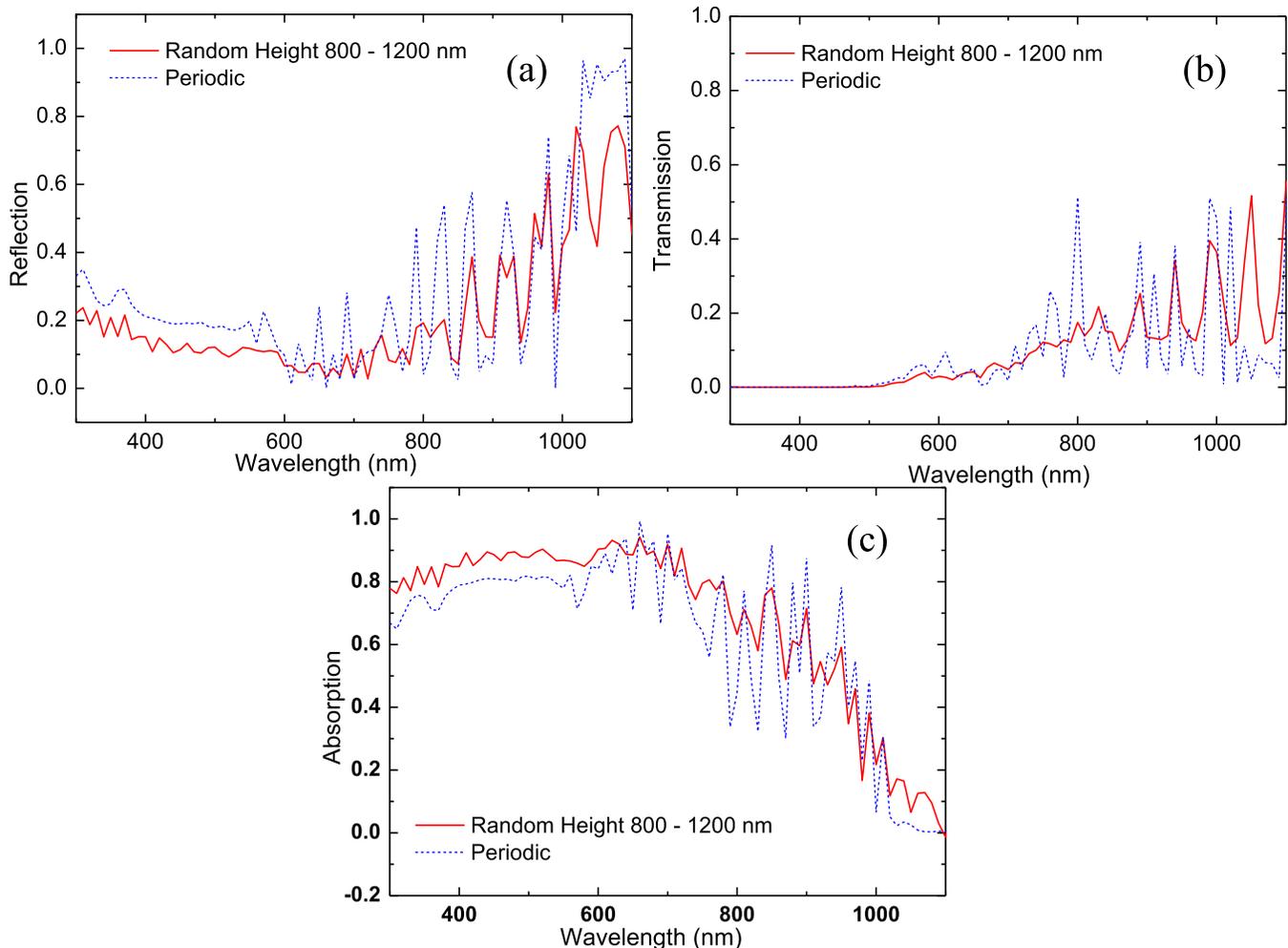

FIG. 4. (a) Light reflection, (b) transmission, and (c) absorption of the SiNH structure with random hole depth.

Frequency Structural Simulator based on the finite element method (FEM).[14] For the simulation, plane wave is incident normally onto the nanostructures with a wavelength λ ranging from 300 nm to 1100 nm. The optical characteristics are obtained by solving the electric field distribution upon the interaction between incident sunlight and the nanohole structures. The refractive index of Si is obtained from the literature.[15] The ultimate efficiency (η) of the RNS is calculated[7,16] and compared with that of the optimum PNS.

III. RESULTS AND DISCUSSION

Figure 3 shows the optical characteristics of the RNS with varying R and compared with those of the optimum PNS. In this case, the hole radius is distributed over 240 nm ± 60 nm, while the hole depth is fixed at 1 μm and the hole is centered in each sub-cell. It can be seen that the RNS has lower reflectance compared to the PNS over the entire wavelength range investigated. In terms of light transmission, it is almost zero for $\lambda < 700$ nm, indicating that most of the light is absorbed before reaching the bottom of the nanohole structure. This is similar to the results observed for the PNS, and indicates that the presence of randomness in the structure does not compromise the light trapping ability of the nanohole structure. On the other hand, it is noted that light transmission is higher for the RNS at longer wavelength of $\lambda > 1000$ nm. However, this part of the solar spectrum is not important for Si as its absorption coefficient is relatively diminished. Nevertheless, due to the lower reflection, overall the absorption in this long wavelength range is still better for the RNS as compared to the PNS, as can be seen in Fig. 3(c). As for the entire solar spectrum considered, it is noted that the RNS generally offers better absorption relative to the PNS. The same is also observed for the structures with random depth and position, as illustrated in Figs. 4(c) and 5(c). Therefore, it is indeed beneficial to have randomness in the SiNH structure as it will help improve light absorption.

As seen in Fig. 3(c), the absorption spectrum of the PNS is noted to be oscillatory for $\lambda > 600$ nm, which indicates the presence of guided modes in the structure. The guided modes refer to those optical modes that can be guided into the nanostructures and result in resonance absorption. This is accompanied by the trapping of light and there is lateral propagation of the trapped sunlight.[17] In contrast, the light absorption spectrum of the RNS is much
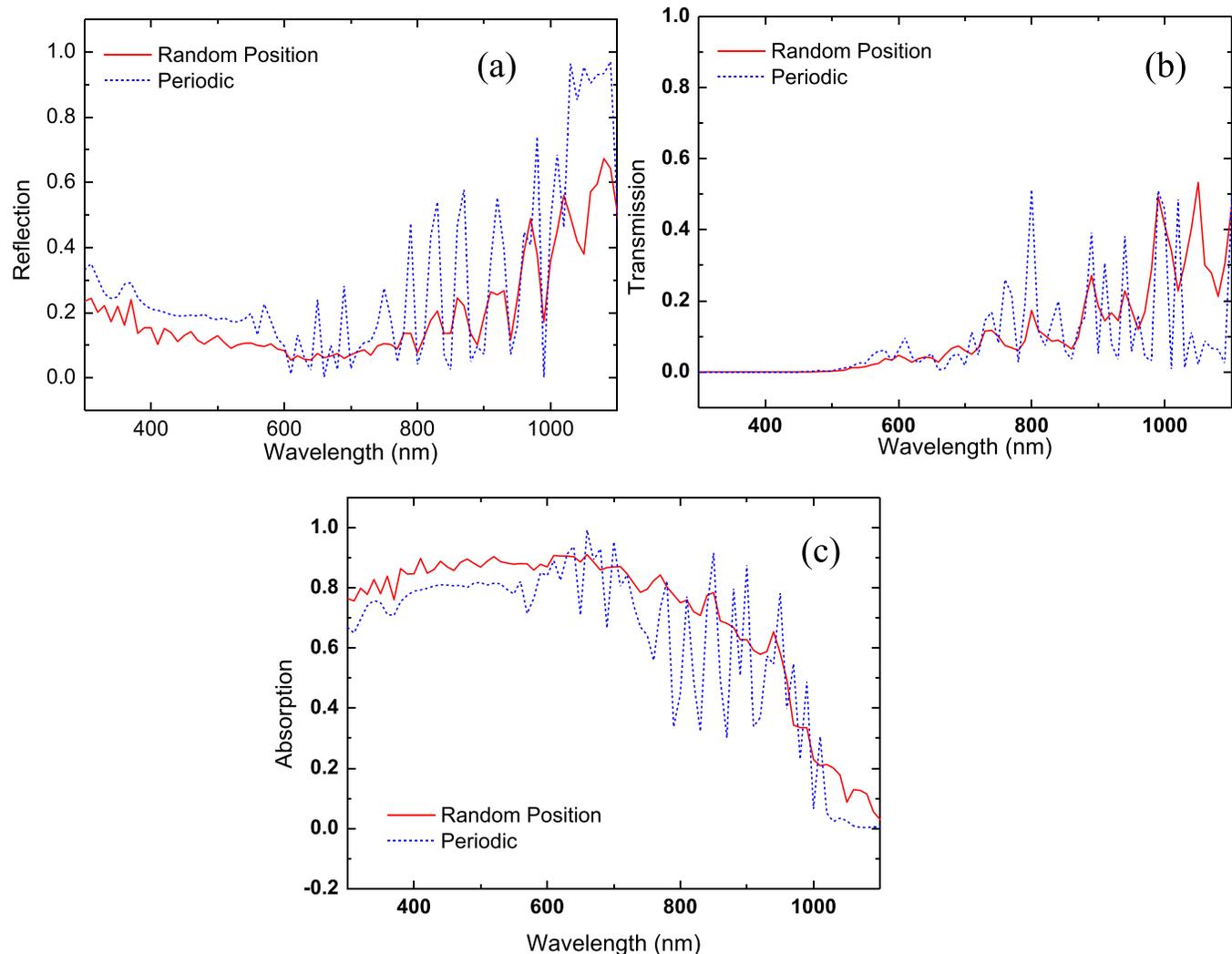

FIG. 5. (a) Light reflection, (b) transmission, and (c) absorption of the SiNH structure with random hole position.

TABLE I. Ultimate and theoretical efficiency of different random silicon nanohole structures.

	Periodic nanohole	Random hole radius	Random hole depth	Random hole position
Ultimate efficiency	30.0%	33.6%	32.9%	33.8%
Theoretical efficiency	13.06%	14.68%	14.37%	14.77%

flatter and stronger, as the structural symmetry is broken by variation in the hole radius.[18,19] Therefore, the structural disorders result in additional resonances and broadening of the existing resonance, and consequently more light coupled into the guiding modes of the RNS and hence enhanced light absorption.[11] Table I shows the ultimate efficiency of the PNS and RNS. The ultimate efficiency of 33.6% for the structure with random R is higher than that of the PNS of 30%, representing an improvement of about 12%. The theoretical efficiency is also calculated using the formula $\eta = J_{sc}V_{oc}\Gamma_f/P_{in}$,[20,21] where J_{sc} is the short circuit current, V_{oc} is the open circuit voltage, Γ_f is the fill factor, and P_{in} is the incident solar power. The same assumptions of fill factor of 80% and carrier collection efficiency of 85% with a 5% shadowing effect are made in our calculation.[20,21] It is found that η is 14.68% for the RNS structure with random radius, which is higher than the 13.06% achieved for the PNS.

Figures 4 and 5 show the optical characteristics of the SiNH structures with random hole depth and position, respectively. For the case of random hole depth, the hole depth is randomly distributed from 0.8 to 1.2 μm, while the hole radius is fixed at 240 nm and the hole is centered in each sub-cell. For the case of random hole position, the center of the hole is randomly displaced from the center of each sub-cell by a maximum of $\pm$ 60 nm, while the hole depth and radius are fixed at 1 μm and 240 nm, respectively. It is found that their light absorption spectra reveal a similar trend as seen earlier for the case of the structure with random hole radius. The light absorption for the RNS is higher than the PNS, and it is also not as oscillatory in the long wavelength range. For the

random hole depth structure, due to the hole depth randomness, the incident light experiences a more gradual change in the effective refractive index. Consequently, due to the better index matching between air and the SiNH structure, light reflection is substantially reduced as seen in Fig. 4(a).[22,23] The ultimate efficiency achieved is 32.9%, which is 9.7% higher compared with that of the PNS. The theoretical efficiency of 14.37% is also higher than that of the PNS. For the case of the structure with random hole position, the ultimate efficiency achieved of 33.8% is also improved compared to that of the PNS. Likewise, the theoretical efficiency of 14.77% is also better than that of the PNS. Since the nanostructures have dimensions that are comparable with the sunlight wavelength, it is possible to have diffraction related enhancement.[24] However, it is not straightforward to separate this from the cavity effect and the guided modes. Comparing the absorption spectra of the PNS and RNS shown in Figs. 3(c), 4(c), and 5(c), it is noted that there exists new resonances modes for $\lambda < 600$ nm in the spectra of the RNS that are not observed for the PNS. The new resonance modes at shorter wavelength can be attributed to the presence of small structures, as the random structures would have some of the structural parameters, such as periodicity and radius, reduced. On the other hand, for $\lambda > 600$ nm, it is seen that the prominent resonance absorption peaks originally associated with PNS have been broadened, as revealed in the spectra of the RNS. This broadening is ascribed to the variations in the structural parameters of the RNS.

Figure 6 shows the ultimate efficiency of the periodic and random nanostructures with random radius and depth at varying incident angles for TE and TM polarized light. It is seen that for the TE polarization, the ultimate efficiency decreases as the incident angle increases for both the PNS and RNS. However, the light absorption is consistently higher for the RNS as compared with the PNS at all the incident angles simulated, indicating better light absorption ability of the RNS. For the TM polarized light, it is observed that the ultimate efficiency decreases and reaches a minimum, before it increases with incident angle for the case of PNS. Again, a higher ultimate efficiency is achieved for the
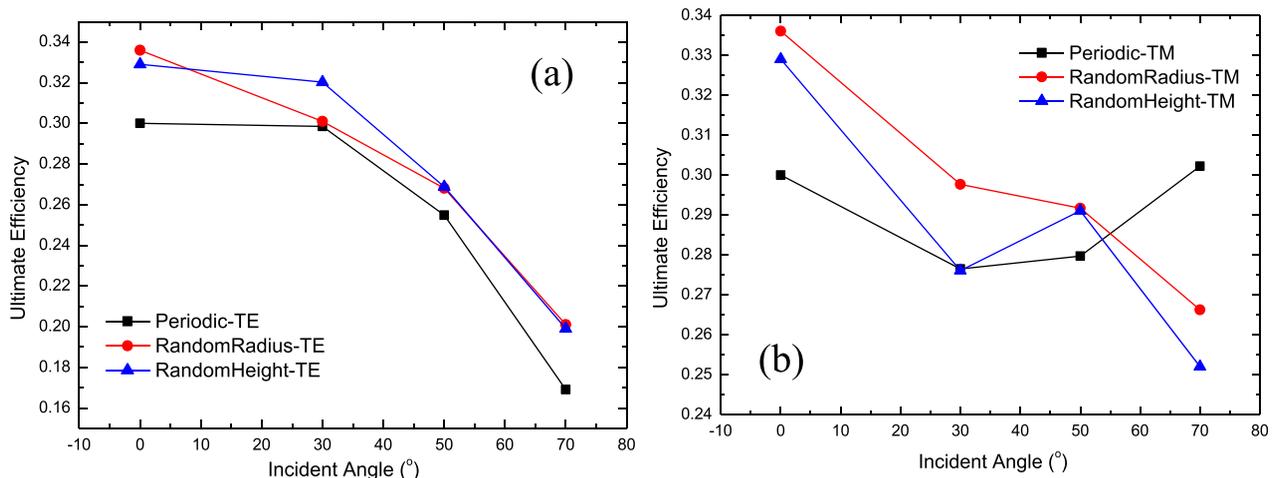

FIG. 6. Angular dependence of the ultimate efficiency of the periodic and random nanostructures with (a) TE and (b) TM polarizations.

RNS as compared with the PNS at different incident angles up to 50°. At larger incident angle of 70°, the ultimate efficiency of the RNS is, however, lower as compared to the PNS. Therefore, it is concluded that for incident angles up to 50°, RNS has better light absorption as compared to PNS for both TE and TM polarization of light. This is encouraging for the practical application of non-periodic SiNH in solar cells for light trapping, fabricated using low cost techniques.

In conclusion, it is noted that generally light absorption is improved for non-periodic SiNH structures with variation in hole radius, depth, and position, as compared to the periodic SiNH structure. This suggests that it is indeed advantageous to use lower cost techniques such as electroless chemical etching with Ag catalyst for the fabrication of such SiNH structures to enhance light absorption. This is important in the attempt to develop low cost and high efficiency Si nanostructures based solar cells.

IV. CONCLUSIONS

In summary, finite element method is used to simulate the optical characteristics of a SiNH structure with randomness introduced into the structural parameters which include the hole radius, depth, and position. The light absorption of the random nanostructures is significantly improved compared to the periodic SiNH structure due to reduced reflection, additional resonances induced and broadening of the existing resonance. Therefore, the structural randomness is beneficial for light absorption in silicon nanohole structure.

ACKNOWLEDGMENTS

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