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# Design guidelines for slanting silicon nanowire arrays for solar cell application

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The reflectance and absorption characteristics of slanting silicon nanowires (SiNWs) structure have been simulated using finite element method to provide a design guideline for its application in solar cell. The slanting angle for the nanowire structure is set at  $40^\circ$  on Si (111) wafer. The impact of the structural periodicity (P) and wire diameter/periodicity (D/P) ratio on the optical characteristics of the slanting SiNW has been systematically analyzed. It has been found that due to the much suppressed light reflection and stronger light trapping ability, the light absorption is significantly enhanced for the slanting SiNW structure compared with vertical SiNW structure. The optimal absorption condition is achieved when  $P=800\text{ nm}$  and  $D/P=0.7$ , yielding the highest ultimate efficiency of 33.45%. The result is better than the 28.36% that can be achieved for optimum vertical SiNWs. A comparison of the absorption characteristics of optimum slanting and vertical SiNWs structures is presented and analyzed in terms of the physical light interaction with the structures. © 2013 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4819175>]

## I. INTRODUCTION

To address the pressing problem of increasing energy shortages and serious environmental pollutions, there has been active research on non-conventional lower cost and higher efficiency solar cells. Among them, solar cells based on silicon nanowires (SiNWs) have gained tremendous interest due to their strong light absorption.<sup>1–4</sup> For example, compared with solar cells based on planar Si wafer, solar cells based on radial SiNW pn junction can effectively decouple light trapping from carrier collection.<sup>5</sup> Correspondingly, the power conversion efficiency (PCE) can be significantly improved by optimizing the optical and electrical parameters of SiNW arrays independently, to enhance light absorption and facilitate carrier diffusion. Currently, ordered SiNW structure can be fabricated using methods like lithography,<sup>6</sup> polystyrene ball assembly,<sup>7</sup> etc. However, the high cost and complexity of these methods render them unattractive. Recently, large-scale SiNW arrays have been successfully fabricated with a simple and low cost maskless approach<sup>8,9</sup> based on the electroless metal catalyst wet etching, with the help of metal nanoparticles catalyst functioning as the etching catalyst for the formation of SiNW structure. This technique has a strong etching direction dependence on the Si crystallography, with a much faster etching speed along the (100) orientation.<sup>10–12</sup> Different SiNW slanting angles have been achieved from silicon wafers with different crystallographic orientations. For example, a slanting angle of  $40^\circ$  has been obtained from Si (111) wafer as demonstrated by Zhang *et al.*<sup>12</sup> In addition, they have shown that the Si (111)

achieved a higher PCE and was easier to control than Si (100) wafer in their application in hybrid Si solar cell.<sup>13</sup> Fang *et al.* have also successfully fabricated solar cell device based on the slanting SiNW structure, and demonstrated an improved light absorption and PCE than the vertically aligned SiNW device.<sup>14</sup> Besides the above, slanting SiNW can be fabricated by controlling the etching solution concentration.<sup>15</sup>

There have been extensive simulation studies conducted to understand the performance of SiNW based solar cells, focusing mainly on vertically aligned SiNW arrays.<sup>3,16</sup> In contrast, simulation studies on the optical characteristics of slanting SiNW are lacking in the literature. In this work, we have performed a systematic simulation of the optical characteristics of slanting SiNWs using the Finite Element Method (FEM) method. The study provides a useful design guideline on the structural parameters of the slanting SiNWs solar cell, namely, the periodicity (P) and diameter (D), which will maximize light absorption. The slanting angle we have chosen for the SiNW is  $40^\circ$ , based on the value reported experimentally for Si (111) wafer.<sup>12</sup> The effects of the parameters P and D on the optical characteristics of the slanting SiNW have been systematically investigated. The light absorption has been found to be substantially improved due to the combined effect of suppressed light reflection and a strong light harvesting ability of the slanting SiNWs. The optimal condition is achieved with a P of 800 nm and D/P ratio of 0.7, measured in terms of the ultimate efficiency. In addition, a comparison of the light absorption spectra between the slanting and vertically aligned SiNW structure is also conducted to understand the differences in their absorption of light. It is found that the slanting SiNW outperforms the vertical counterpart by  $\sim 18\%$  in terms of light absorption. Therefore, the slanting SiNWs structure presents an effective way to improve the PCE of SiNW based solar cell devices.

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## II. SIMULATION METHODOLOGY

Figures 1(a)–1(c) illustrate the schematic of the simulated slanting SiNWs in three dimensional, top and cross-sectional views respectively, and Figure 1(d) shows the cross-sectional view of the vertically aligned SiNW for comparison. The slanting angle is chosen to be  $40^\circ$  based on the experiment result reported for Si (111) wafer.<sup>12</sup> The vertical height ( $H$ ) of the slanting SiNW is  $1\ \mu\text{m}$  and the underlying Si thin film is  $1\ \mu\text{m}$  thick. The two parameters,  $D$  and  $P$ , are varied to find the optimal geometric configuration for optimum light absorption. Light with wavelength ranging from  $300\text{ nm}$  to  $1100\text{ nm}$  is incident normally on the surface of the nanostructure. The optical constants of Si used in the simulation are taken from the literature.<sup>17</sup> Finite element method is used to account for the interaction between the incident light and the SiNW structure using the High Frequency Structural Simulator software.<sup>18</sup> The spatial distribution of the electric field is determined and based on which the optical characteristics of the structure can be calculated.

In order to evaluate the light absorption ability and the optimal absorption condition, the ultimate efficiency ( $\eta$ ) of the structure is calculated as follows by weighing the absorption spectra over the AM 1.5G solar spectrum,<sup>16,19</sup> assuming that the internal quantum efficiency is 1

$$\eta = \frac{\int_{300}^{1100} \frac{E_g P(\lambda) A(\lambda)}{E} d\lambda}{\int_0^\infty P(\lambda) d\lambda}. \quad (1)$$

In the above,  $E_g$  is the band gap of Si,  $E$  is the photon energy of incident sunlight,  $\lambda$  is the wavelength of the incident light,  $A(\lambda)$  is the absorption efficiency at each wavelength, and  $P(\lambda)$  is spectral irradiance of the standard AM1.5G solar spectrum at each wavelength.

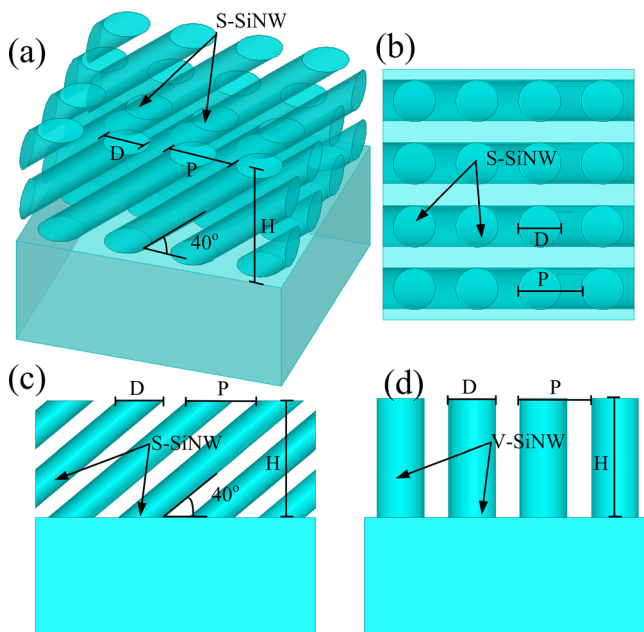


FIG. 1. Schematics illustration of the slanting SiNW with (a) three-dimensional view, (b) top and (c) cross-sectional views, and (d) of the cross sectional view of the vertical SiNW.

## III. RESULTS AND DISCUSSION

Figure 2 shows the absorption spectra of the slanting SiNWs with a fixed  $D/P$  ratio of 0.7 for different  $P$ . When  $P$  is  $400\text{ nm}$ , the absorption is high at shorter  $\lambda$  because the wavelength is comparable with the  $P$  of the SiNW, leading to stronger scattering of light and inducing stronger light absorption.<sup>3,20</sup> The absorption is noted to decrease substantially for  $\lambda > 600\text{ nm}$  since the wavelength is much larger than the dimension of the slanting SiNW structure and hence light will easily penetrate through the film without significant interaction with the SiNW structure, leading to a poor absorption. As  $P$  increases to  $600\text{ nm}$ , the absorption is slightly reduced at shorter  $\lambda$  and improved for light ranging from  $600\text{ nm}$  to  $800\text{ nm}$ , attributed to the same reason as explained above. Similarly, when  $P$  is  $800\text{ nm}$ , the absorption is further increased for longer  $\lambda$  beyond  $800\text{ nm}$ . The optical path length of the light is substantially extended due to enhanced scattering, which is particularly important for longer wavelength light that has a weaker absorption in Si. Therefore, a high and broadband light absorption is achieved at  $P = 800\text{ nm}$ . In fact, as  $P$  increases, the light absorption edge will shift towards longer wavelength light region, meanwhile, the increased  $P$  will result in a higher reflectance, especially for short wavelength light. Hence, those two effects will compete as  $P$  increases. At  $P = 900\text{ nm}$ , the dimension of the structure (structural periodicity) is larger than majority of the sunlight of interest. Hence, the interaction between short wavelength light and the slanting SiNW structure is weaker. Hence, the light reflection and light transmission increase a little bit compared with that of  $P = 800\text{ nm}$  for  $\lambda < 900\text{ nm}$ . Therefore, those effects contribute to a drop in light absorption for  $P = 900\text{ nm}$ . In summary, the optimal structural periodicity is achieved at  $P = 800\text{ nm}$ .

With  $P$  fixed at  $800\text{ nm}$  while the  $D/P$  ratio is varied, the optical characteristics exhibit a trend similar to what has been observed in Fig. 3 in terms of the relation between the dimension of the structure and the wavelength of light. For small  $D/P$  ratio of 0.5, the wire diameter is  $400\text{ nm}$  and hence light absorption is much higher for shorter  $\lambda$  due to the stronger scattering between sunlight and wire structure. However, the absorption is lower for longer wavelength light with  $\lambda > 600\text{ nm}$ . As the  $D/P$  ratio increases to 0.6, the absorption is improved at longer  $\lambda$  but is decreased slightly at shorter  $\lambda$ . At the  $D/P$  ratio of 0.7, the reflection is further reduced for longer  $\lambda$  and there is also a drop in transmission, resulting in high absorption over the solar spectrum from  $300\text{ nm}$  to  $1100\text{ nm}$ . When the  $D/P$  ratio is further increased to 0.8, the reflection increases significantly for  $\lambda < 600\text{ nm}$  and the transmission is also increased compared to that of 0.7. Therefore, the overall light absorption degrades. The maximum absorption is hence achieved at the optimal  $D/P$  ratio of 0.7.

Figure 4 depicts the ultimate efficiency  $\eta$  and the maximum short circuit current density<sup>21</sup> for different  $P$  as a function of the  $D/P$  ratios. The maximum short current density can be calculated based on the value of ultimate efficiency by assuming each generated carrier will be collected at the electrodes and contribute to the current.<sup>21</sup> The trends for the two parameters are the same. It is observed that for all  $P$  values,  $\eta$  increases initially with the  $D/P$  ratio, reaches a

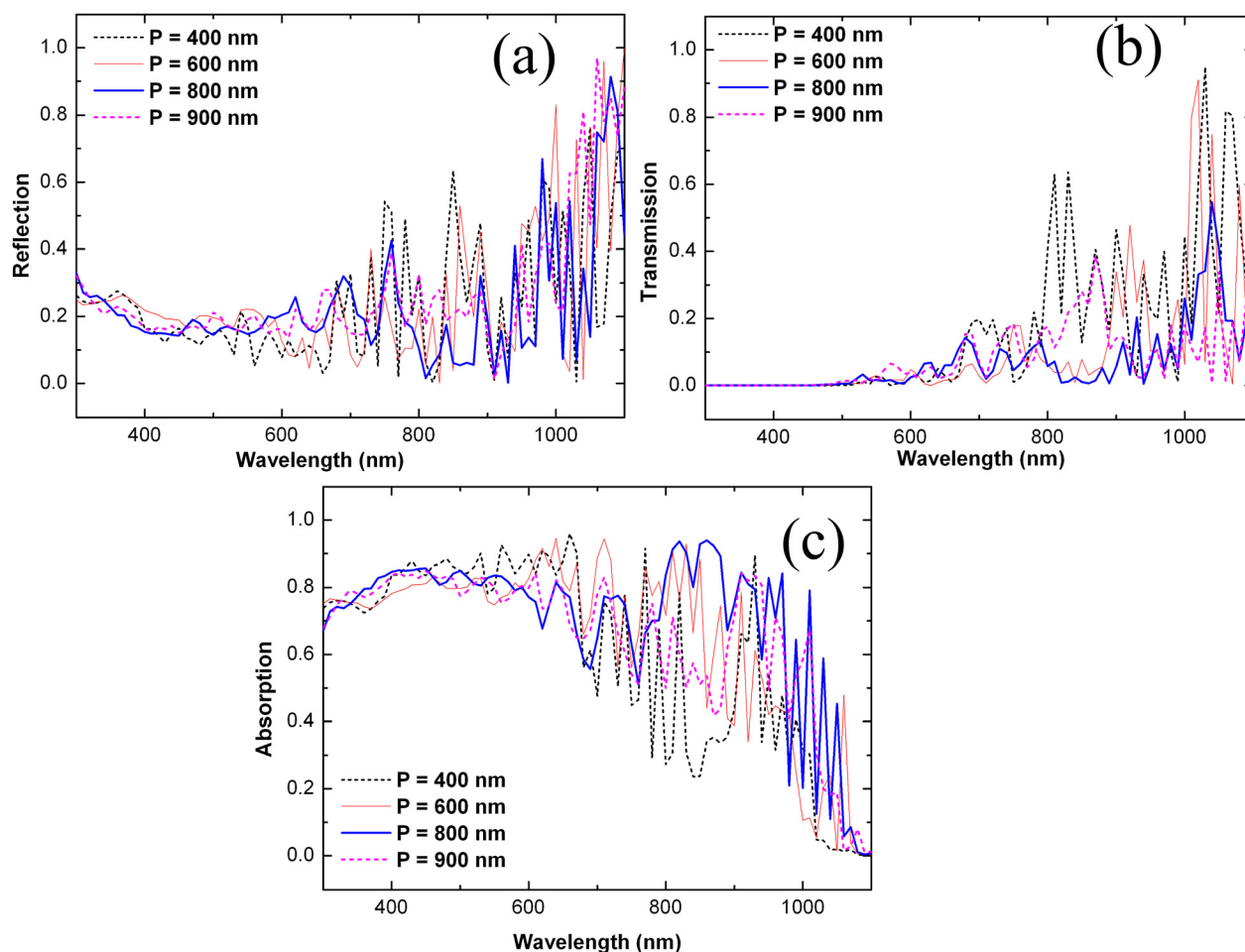


FIG. 2. (a) Reflection, (b) transmission, and (c) absorption spectra of the slanting SiNW structure with a fixed D/P ratio of 0.7 for different periodicities.

maximum and then decreases at larger D/P ratio. The optimized D/P ratios for different P are generally located at around 0.6 to 0.8, indicating a wide D/P ratio window where light trapping is enhanced. For D/P ratio  $< 0.5$ , the structure does not induce strong light scattering, and therefore the  $\eta$  is low. On the other hand, for slanting SiNW with a D/P ratio large than 0.8, its structure is similar to a planar film with a much reduced light harvesting ability. It is noted that for small P of 300 nm the  $\eta$  is generally low since the wire diameter is much smaller than the wavelength of light of the solar spectrum. As P increases, there is an increase in  $\eta$  and it is observed that the optimum  $\eta$  for P from 600 to 800 nm are comparable. This indicates that there is a wide window of structural periodicity that can give rise to strong absorption enhancement. Therefore, both the wide windows of the D/P ratio and the P to achieve a high  $\eta$  suggest a large tolerance allowed for the fabrication process. The highest  $\eta$  of 33.45% is achieved when P is 800 nm with a D/P ratio of 0.7. It is higher than that of its vertical counterpart SiNW structure, which has the highest ultimate efficiency of 28.36%. In terms of the current density, the highest value achieved is  $\sim 27.37 \text{ mA/cm}^2$ . Therefore, it indicates that the slanting SiNW structure has better light absorption ability than the vertical SiNW structure.

Figure 5 compares the optical characteristics of the optimized slanting and vertical SiNWs structures, as well as

those of a planar  $2 \mu\text{m}$  thin film. The optimal structure for the vertical SiNW occurs at a P of 600 nm and D/P ratio of 0.65. Compared with the planar film, both the slanting and vertical SiNWs structures exhibit a much lower light reflection and transmission, and hence stronger light absorption. As for the two SiNWs structures, when measured using the ultimate efficiency, the slanting structure displays a light absorption that is  $\sim 18\%$  higher compared with the vertical structure. A comparison reveals that for  $\lambda < 550 \text{ nm}$ , the absorption of the vertical and slanting SiNWs structures is similar. Whereas for  $\lambda$  in the range of 600 nm–800 nm, the vertical structure has a stronger light absorption due to enhanced light scattering, since the optimum P is 600 nm. For  $\lambda > 800 \text{ nm}$ , both the reflection and transmission of the slanting SiNW are observed to decrease and correspondingly the light absorption is significantly improved compared to the vertical structure.

The differences observed between the vertical structure, slanting structure, and the planar thin film can be explained as follows in terms of the changes in refractive index and the trapping of light. For the planar film, the abrupt change of the refractive index between air and silicon induces a large reflection. For the vertical and slanting structures, the SiNWs function as a homogeneous antireflective layer between air and Si. As a result, there is better refractive index matching which leads to a suppression of light reflection.<sup>22,23</sup> On the

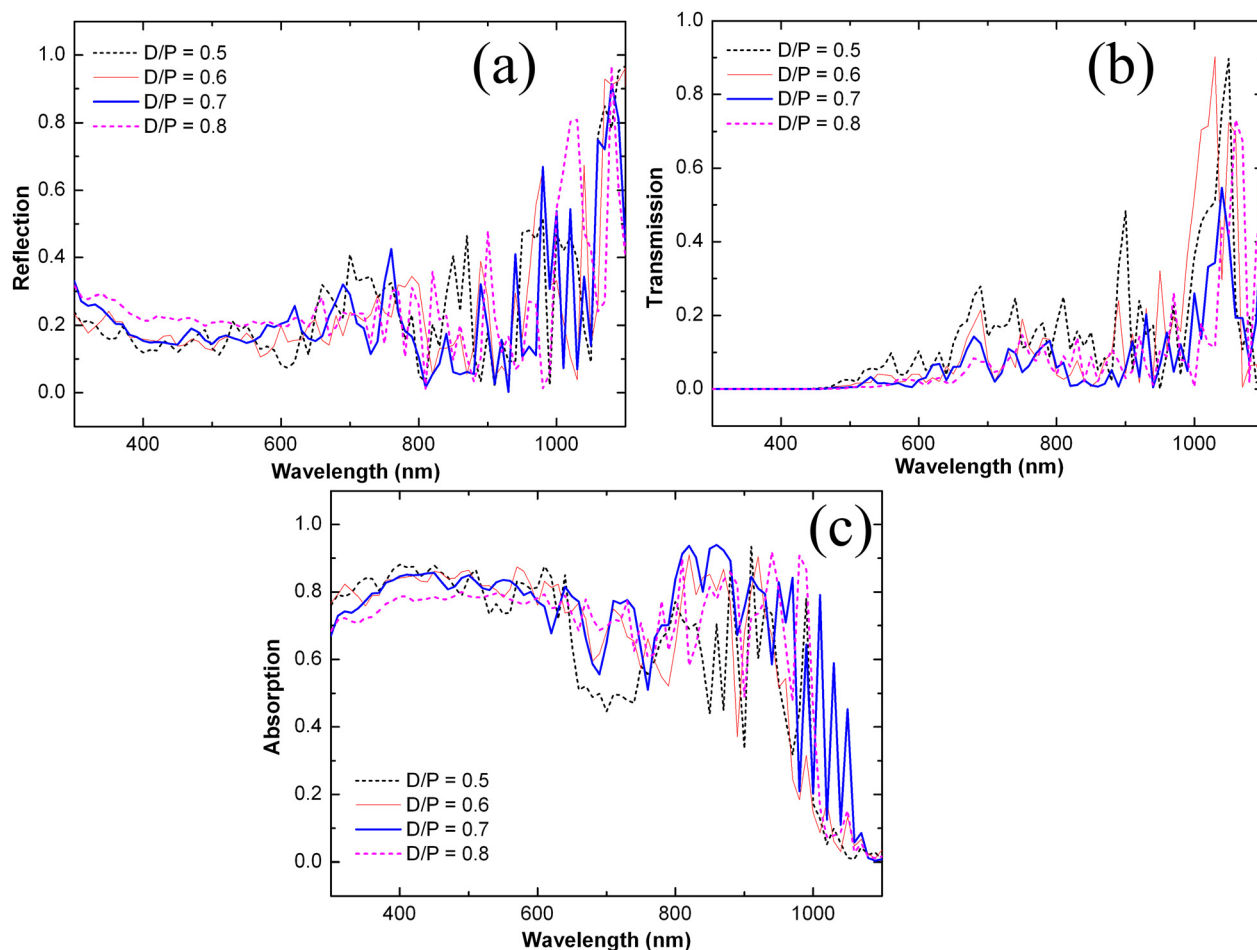


FIG. 3. (a) Reflection, (b) transmission, and (c) absorption spectra of the slanting SiNW structure with a fixed periodicity of 800 nm for D/P ratio.

other hand, in terms of trapping of light, it does not exist for the planar Si film. Though this exists for the vertical SiNWs, however, due to the symmetrical property, there is a degeneracy of the modes,<sup>24,25</sup> leading to a decrease of light absorption. By the introduction of the slanting SiNW, the mirror symmetries are reduced from four for the vertical SiNWs to only one for the slanting SiNWs.<sup>24,25</sup> Therefore, more light

can be coupled into the guiding modes of the structure resulting in stronger light absorption. In summary, the slanting SiNWs structure demonstrates a strong suppression of light reflection and enhanced light trapping ability, rendering it attractive for application in thin film solar cells. Note that the design principles presented here are not restricted to Si, but can be applied to other solar cell materials.

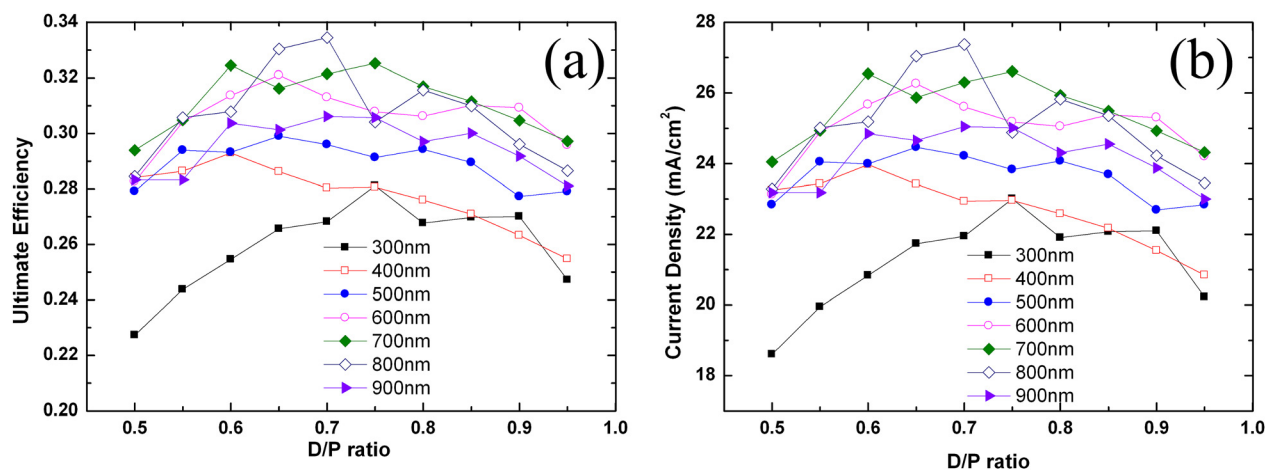


FIG. 4. (a) Ultimate efficiency and (b) maximum short circuit current density of the slanting SiNW structure at different periodicities with varying D/P ratio.

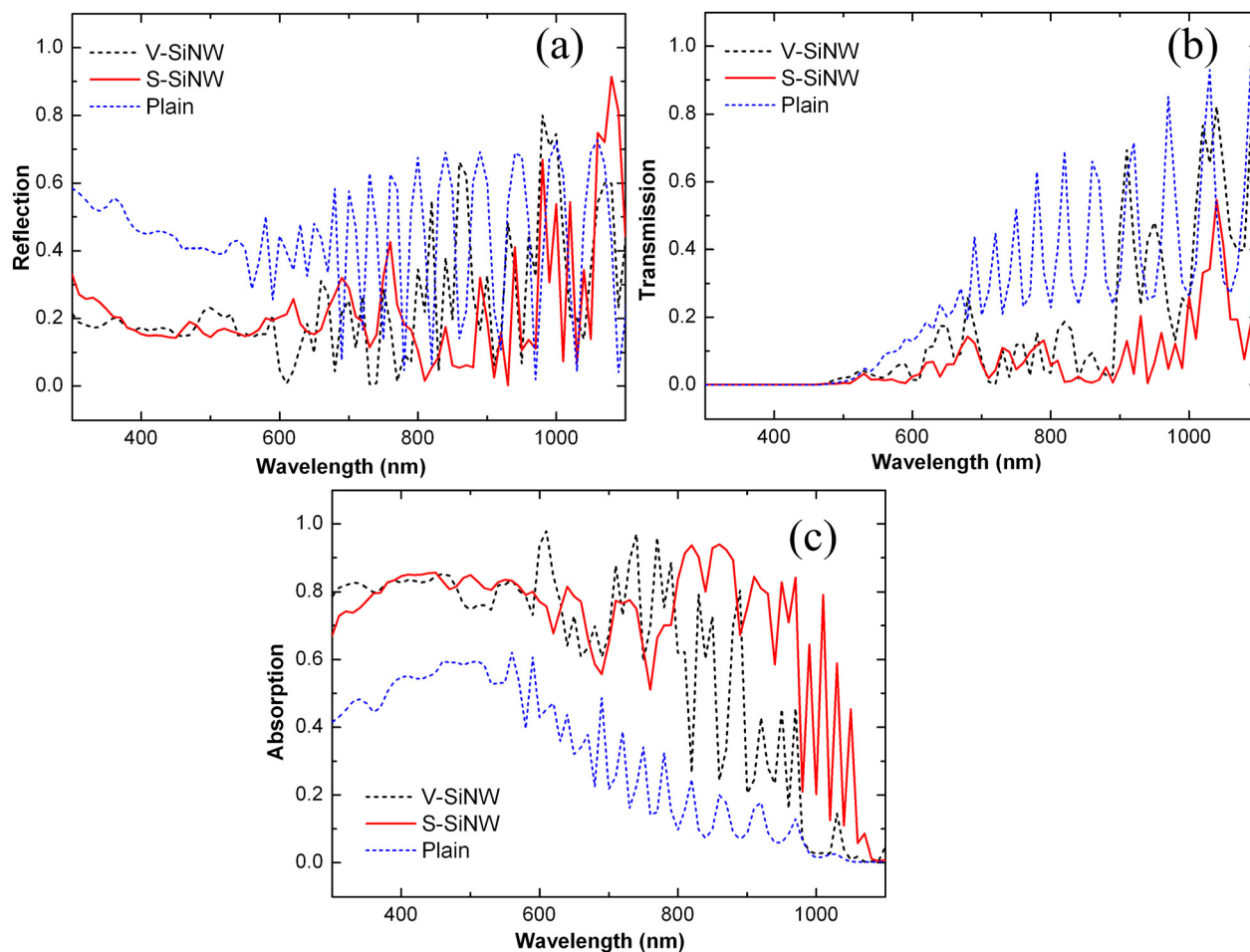


FIG. 5. (a) Reflection, (b) transmission, and (c) absorption spectra of the optimal slanting, vertical SiNW, and the planar 2  $\mu\text{m}$  thin film.

#### IV. CONCLUSIONS

In summary, the effects of structural periodicity and wire diameter of slanting SiNWs on the light absorption have been systematically analyzed. The optimal geometrical configuration is achieved when the periodicity is 800 nm and diameter/periodicity ratio is 0.7, which gives rise to the highest ultimate efficiency of 33.45%. This is higher than that of optimized vertical SiNWs structure, which has a highest ultimate efficiency of only 28.36%. The slanting structure proposed offers better suppression of light reflection and light harvesting ability than the vertical structure, and potentially can further improve the performance of SiNWs based solar cells.

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