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Light-trapping properties of the Si inclined nanowire arrays

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ABSTRACT

The light trapping performance of Si nanowire with different inclination angles were systematically studied by COMSOL Multiphysics. The inclined nanowires with inclination angles smaller than 60° show greater light trapping ability than their counterparts of the vertical nanowires. The Si solar cell with the inclined nanowires of the optimal parameters, whose $\theta=30°$, $P=400$ nm, $D=140$ nm, can achieve a 32.395 mA/cm^2 short circuit photocurrent density and a 35.655% conversion efficiency. The study of the inclined nanowire provides an effective way for further utilization of the incoming light.

1. Introduction

Photovoltaics is popularized at a rapid speed and has a promising outlook. More and more solar panels are installed in power plants, commercial premises, and residential houses [1,2]. Thin film solar cell, with better flexibility, lighter weights, less usage of raw material, cheaper processing and ease of integration, gains larger proportion in the solar cell market [3]. However, light management and carrier management are still two main problems [4]. The decrease in thickness may also be accompanied by incomplete absorption of photons and a corresponding decrease in efficiency. Nanowire is widely used in improving the light management duo to their unique optical properties and compatibility with inexpensive fabrication techniques. As the light trapping ability is sensitive to the morphology of the nanowire structure, the nanowires' diameter, period and ratio of diameter/period have been extensively studied both theoretically and experimentally to boost the light harvesting ability of the solar cells [5–9]. The major preparation methods of nanowires include etching by acid solutions, oblique angle deposition (OAD), molecular beam epitaxy (MBE), vapor-liquid-solid(V-L-S), reactive ion etching (RIE) etc. Apart from the vertical nanowires (VNW), inclined nanowires (INW) with varying inclination angles are obtained [10–13]. To our knowledge, there are insufficient studies to investigate the inclination angles of Si inclined NW on light trapping so far. In this paper, systematic simulations were conveyed by COMSOL Multiphysics to study the light harvesting ability of INW. The results reveal that the Si INW arrays outperform the vertical counterpart in certain angle range.

2. Methods

By employing Maxwell equations, the COMSOL Multiphysics is widely used in the analysis of the electromagnetic wave propagation in the nanostructures. Air Mass 1.5G (AM 1.5G) was used. Perpendicular incident light (the propagation direction was along the -z direction) of transverse electric (TE) and transverse magnetic (TM) wave were calculated separately. TE polarized plane wave had its electric field along the -y direction, while TM polarized case had its electric field in the x direction. Simulations were carried out at the wavelength regime of 310–1127 nm with a 5 nm step size, which is the corresponding wavelength range of the Si band gap. The silver back reflection layer was added to reduce the light transmission. To model the periodic array structure, the simulations were carried out by introducing the periodic boundary conditions (PBC) in both the $\pm x$ and $\pm y$ directions (the PBC in the -y direction is not shown in Fig. 1(a) to have a clear view of the model) [14]. To model a semi-infinite Si substrate, the periodic match layer (PML) was added in the vertical direction, which the transmission light was totally absorbed [15]. The short current density and efficiency are denoted as J_{sc} and η respectively [16,17].

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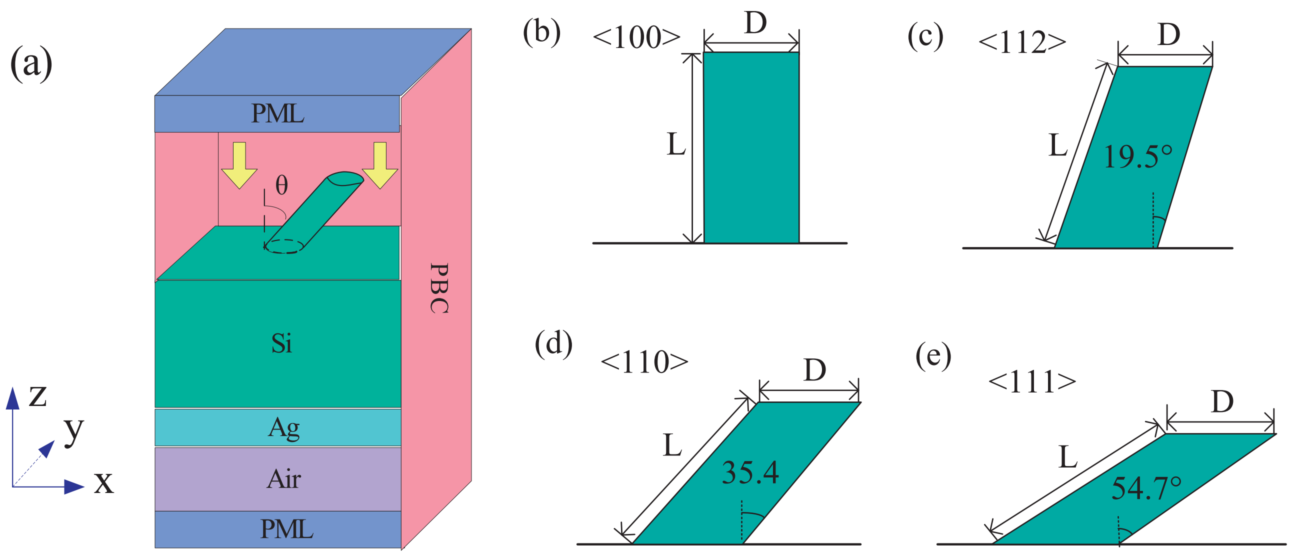

Fig. 1. The diagram of the model, the nanowires are 500 nm in length and on the silicon substrates of 1 μm thick (a), nanowires with the orientation of < 100 > (b), < 112 > (c), < 110 > (d), < 111 > (e).

$$J_{sc} = \int_{310\mathrm{nm}}^{\lambda_g} I(\lambda)A(\lambda)\frac{e\lambda}{hc}d\lambda \tag{1}$$

$$\eta = \frac{\int_{310\mathrm{nm}}^{\lambda_g} I(\lambda)A(\lambda)\frac{\lambda}{\lambda_g}d\lambda}{\int_{310\mathrm{nm}}^{4000\mathrm{nm}} I(\lambda)d\lambda} \tag{2}$$

where λ_g is the corresponding wavelength of the Si band gap, i.e. 1127 nm, $I(\lambda)$ is the standard solar irradiance spectrum of AM1.5 G, $A(\lambda)$ is the optical absorption of the structure at the wavelength λ, e is the elementary charge, h is the Planck constant, c is the velocity of light in vacuum.

The cross sectional view of the model is depicted in Fig. 1, the VNW and INW Si nanowire arrays on crystalline silicon substrates were devised for comparative analysis. As is illustrated in Fig. 1(b)–(e), comparative simulations were made between the vertical (< 100 > -oriented) and inclined NWs with growth direction along three common crystal orientation of silicon (< 110 >, < 111 > and < 112 >). The corresponding parameters are labeled clearly, where θ is the inclination angle to the vertical direction. When θ equals 0°, it is the VNW array. D, L and P are the diameter, length and period of the nanowires respectively. The diameter is taken to be $D=100$ nm, the length is set to $L=500$ nm and the period is fixed at $P=600$ nm. All the NWs are on the silicon substrates of 1 μm thick.

3. Results and discussion

3.1. The effect of inclination angle on the Si INW light-trapping ability

The absorption diagrams of the NWs are sketched in Fig. 2. The diameter and period of the NW are fixed at 100 nm and 600 nm respectively. For the INW, the discrepancy of the absorption between TE and TM polarized light results from the anisotropy in the x–y plane of the NW. That differs from the VNW, which the absorption has no obvious difference between TE and TM for it is not sensitive to polarization [18]. The INW shows no obvious advantage over the VNW for the TE polarized light. However, apparent from Fig. 2(b) of the TM-absorption, it's totally a different case. The INW Absorption-TM curves are almost uniformly higher than the VNW of the consistent parameters throughout the

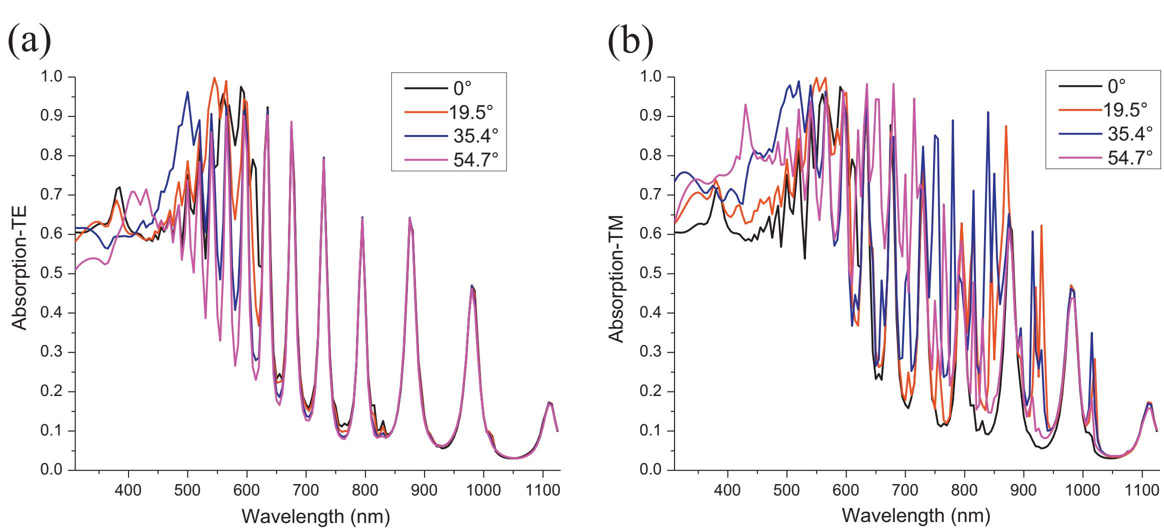

Fig. 2. Absorption of NW with four different inclination angles (vertical, < 110 >, < 111 > and < 112 > -oriented) as a function of wavelength, TE (a) and TM (b).

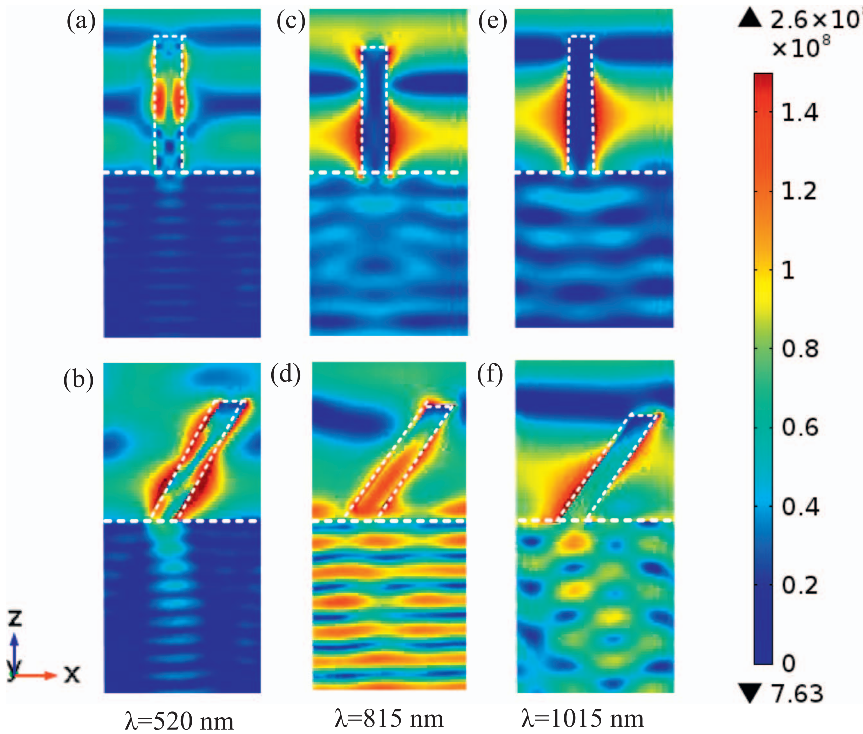

Fig. 3. The intensity distribution of the time-averaged TM polarized electric field at different wavelengths within the VNW ((a),(c),(e)), and the INW with θ=35.4°((b),(d),(f)). The structures are roughly sketched by the dotted line.

broadband wavelength of silicon, resulting from an enhanced optical antenna effect for each NW in TM polarization, which agrees with a previous theoretical work [19]. Particularly, the $<110>$-oriented (θ=35.4°) NW show significant absorption enhancement in the short wavelength region (<550 nm), even climbs almost 100% absorption at some wavelengths. And, it dramatically boosts up for certain wavelengths in 700–900 nm, which substantially strengthen the light-harvesting capability of the solar cells. Furthermore, from Fig. 2, it is noticeable that the resonance peaks show greater inclination angle dependence of TM polarization than that of TE polarization.

That the INW arrays are superior to their companion might be explained by their unique geometry. The electromagnetic wave reflects off one inclined NW surface onto another inclined NW, thus it facilitates the sunlight to make several turns and travel horizontally for distances much longer than that in the VNW arrays. The increase in the effective optical path length results in the maximized light harvesting. This can be verified by Fig. 3, where the electric field distribution map are illustrated. Compare Fig. 3(a) with Fig. 3(b), we can find that the electric field distribution of the INW has a clear overlap with the Si substrate, which means much the light resonantly confined in the arrays could couple into the Si substrate. Thus the strong interaction with the incident light enable the cells to strongly capture the incident light. The unabsorbed long-wavelength light interferes with the reflected light from the top layer of the device and obvious Fabry–Perot interference fringes arise in the Si substrate at wavelength 815 nm (Fig. 3(d)) [20]. Compared with Fig. 3(e), stronger and more complex electric field distribution is observed within the substrate in Fig. 3(f), indicating enhanced light scattering and capturing of the INW arrays [18,21]. This is probably because there are 2nd and 3rd chances for light to enter the silicon cell after the sunlight bounces back and forth within the inclined NWs. With certain inclination angles, the properties of the INW are more complicated and different from the vertical ones. But overall, the electric field intensity among the INWs is relatively higher than that of the VNW arrays at the same wavelength, thus yields a better light entrapment.

On the other aspect, for normal incidence light, nanostructures of low symmetry outperform those of high symmetry. The reason is that perpendicular incident light has an even modal profile, while the symmetric structures have odd and even resonant modes. Therefore only half of the modes of the incident light can have the possibility to couple into the symmetric structures. The symmetry-breaking INW can couple more incoming light into solar cells, which is predicted to provide stronger absorption enhancement at normal incidence [22–25]. Z. Ruan et al. also demonstrated that by breaking the centrosymmetry geometry cross section of the NW, the noncentrosymmetric radiation pattern of the leaky mode resonance (LMRs) could be got, which greatly contributed to enhance light absorption under the half-space illumination [26]. According to the previous work of Brongersma et al. [27], the first-order LMRs exhibit significant change with the angle (refers to the angle between the incident light and the NW), while the second-order LMRs show the weakest angle dependence. So the different angle dependence between TE and TM polarization mentioned above might be explained as follows. The first-order LMRs take up a great share in the TM-absorption of the sunlight, so resonance peaks show strong angle dependence of the TM polarization; on the contrary, the second-order LMRs account for a large proportion in the TE-absorption of the sunlight, so resonance peaks display weak angle dependence of the TE polarization.

To get a deep insight on the behavior of the INW, the inclination angle θ was systematically altered. Keeping the other parameters the same, change the inclination angle from 5° to 85° with an interval of 5°. As is illustrated in Fig. 4(a), the final short circuit current density and conversion efficiency can be got by taking the mean value of TE and TM absorptions into Eqs. (1) and (2). Compared with the VNW, remarkable enhancements can be observed both in the short circuit current density and the ideal efficiency of the INW in small inclination angles. The two mentioned curves

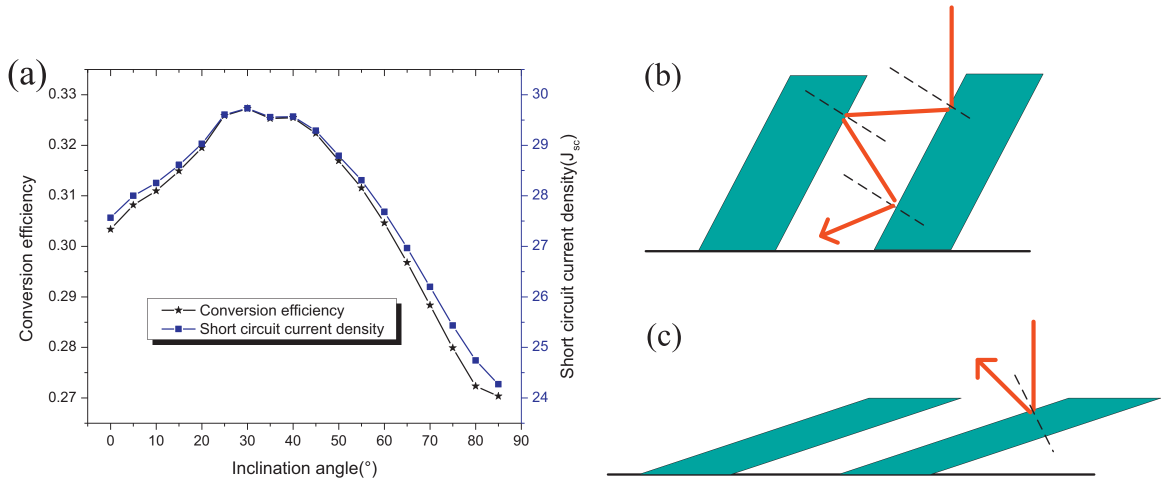

Fig. 4. The short circuit current density and conversion efficiency of INW with different inclination angles. The diameter and pitch are fixed at 100 nm and 600 nm respectively (a).The optical path in the INW of small (b) and large inclination angles (c).

exhibit similar parabola trend, which climb with the growing inclination angle and peak at $\theta=30°$, resulting in a 29.7316 mA/cm^2 short circuit current density (VNW: 27.5641 mA/cm^2) and a 32.723% conversion efficiency (VNW: 30.338%). But the values fall down thereafter, where the INW is inferior to the VNW for angles larger than 60°. The aforementioned phenomena probably can be explained by that for larger angles the normal incidence light reflect out of the NW directly instead of being reflected again among the NWs. Fig. 4(b)–(c) can help to understand the mechanism responsible for this. Besides, comparing with the isolated VNW structure, the proposed INW structure is more mechanically robust and interconnected, which offers excellent carrier transport within the structure [28].

3.2. *The effect of period and diameter on the Si INW light-trapping ability*

As the light absorption is quite sensitive to the geometric parameters, the INW ($\theta=30°$) of different diameters and periods were studied systematically to further optimize the light trapping performance of the device. The *P* and *D* were varied respectively, from 400 nm to 700 nm for the period, from 80 nm to 140 nm for the diameter.

The absorptions of the INW with different periods (*D* is fixed at 100 nm) are plotted as the function of the wavelength in Fig. 5(a). The corresponding short circuit current density and conversion efficiency are shown in Table 1. In the short wavelength range of 310–500 nm, the light trapping performance degrades with the increase of the period. For wavelength regime larger than 500 nm, the absorption curves are almost unaltered for INW of different periods, illustrating the change in period has unpronounced effect on the light trapping ability in the long wavelength. The INW with a period of 400 nm achieves the most efficient absorption. Especially, absorptions around wavelength of 500 nm climb close to 100%, inducing stronger interaction with the incoming light. The INW with period of 600 nm and 700 nm show roughly the same absorption performance.

Meanwhile, the absorptions of the INW with different diameters (*P* is fixed at 400 nm) are portrayed as Fig. 5(b). As the diameter increases, the absorption shows significant improvement accordingly and this is particularly true for short wavelengths. Generally, the INW of 140 nm in diameter shows the obvious

Table 1
The short circuit current density and conversion efficiency of the INW, the diameter *D* is fixed at 100 nm.

D (nm)	*P* (nm)	J_{sc} (mA/cm^2)	η (%)
100	400	29.732	32.723
100	500	29.587	32.564
100	600	28.852	31.755
100	700	27.041	29.020

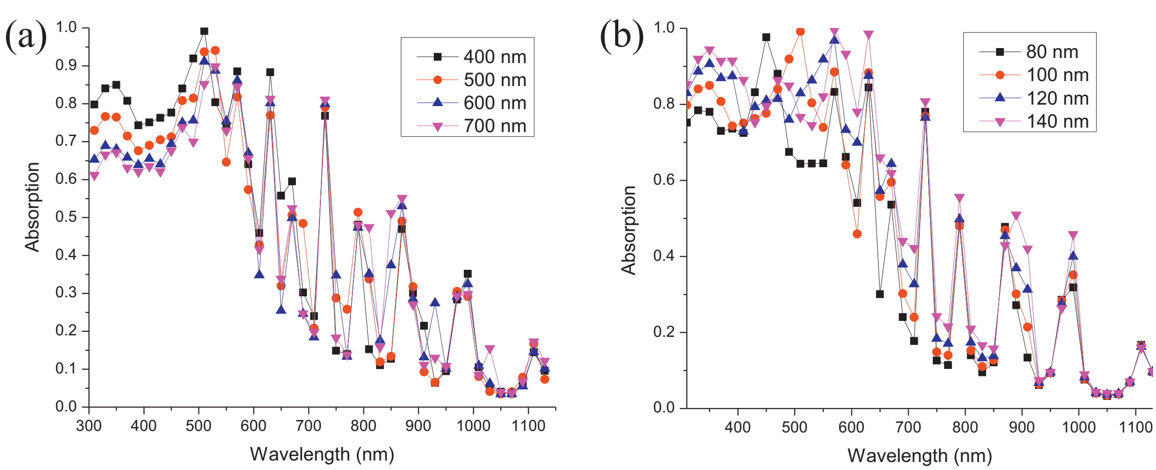

Fig. 5. Absorption of the INW with different periods, the diameter *D* is fixed at 100 nm (a), absorption of the INW with different diameters, the period *P* is fixed at 400 nm.

Table 2
The short circuit current density and conversion efficiency of the INW, the period P is fixed at 400 nm.

P (nm)	D (nm)	J_{sc} (mA/cm^2)	η (%)
400	80	27.905	30.713
400	100	29.587	32.564
400	120	31.060	34.186
400	140	32.395	35.655

advantage against its counterparts. The high absorption can be maintained over a broad spectral band, which contributes to yield a 32.395 mA/cm^2 short circuit current density and 35.655% final efficiency (shown in Table 2). The results of the VNW with the same parameters are 30.338 mA/cm^2 and 27.564% respectively, accounting for an approximately 2 mA/cm^2 improvement in J_{sc} and a near 8% gain in the conversion efficiency.

4. Conclusion

In summary, a systematic study was conducted by Comsol Multiphysics to illustrate the effect of the INW inclination angles on light trapping ability. The changing in inclination angle provides an additional parameter to alter the nanowire morphology. The unique geometry of the inclined NW maximizes the light trapping by making the available sunlight bounced back and forth within the INW and coupled into the substrate, thus significantly contribute to the short circuit current density and conversion efficiency finally. The crystalline silicon solar cell of 1 μm thick patterned with INW of the optimal parameters (θ=30°, P=400 nm, D=140 nm) can yield a 32.395 mA/cm^2 short circuit photocurrent density and a 35.655% efficiency, accounting for approximately 8% efficiency enhancement in comparison with the VNW of the consistent parameters. During the practical preparation procedure, we can get INW with favorable inclination angles or growth direction by regulating the concentration or mixture ratio of the acid solutions, or adjusting the inclination angles when introducing the oblique angle deposition etc. The light trapping ability can be further regulated by modifying the material, inclination angle, geometric dimensions etc. Further analysis are expected in the subsequent researches.

Acknowledgments

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