APPLIED PHYSICS LETTERS **95**, 243113 (2009)

Design guidelines of periodic Si nanowire arrays for solar cell application

Junshuai Li,[1,2] HongYu Yu,[1,2,a] She Mein Wong,[1,2] Xiaocheng Li,[1] Gang Zhang,[2]
Patrick Guo-Qiang Lo,[2] and Dim-Lee Kwong[2]
[1]*School of Electrical and Electronic Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore*
[2]*Institute of Microelectronics, A*STAR (Agency for Science, Technology, and Research), Science Park II, Singapore 117685, Singapore*

(Received 9 November 2009; accepted 25 November 2009; published online 18 December 2009)

In this letter, optimum periodic Si nanowire (SiNW) arrays are designed via simulation for solar cell application, in terms of the structural parameters, e.g., the array periodicity (P) and SiNW diameter (D). It is found that the more efficient light absorption compared to that of the Si thin film with the same thickness could be realized when P is between 250 and 1200 nm. Further, the ratio of D to P should be >0.5 (or more specifically ~ 0.8) for the optimized solar energy harvesting. The underlying physics is also discussed in this work. © *2009 American Institute of Physics*. [doi:10.1063/1.3275798]

Thanks to their uniquely combined optical and electrical characteristics, Si nanowire (SiNW) arrays have received considerable attention for solar cell application.[1–6] Especially low grade Si raw materials can be utilized when integrating the SiNW arrays, as the light absorption and photogenerated carrier extraction processes can be decoupled,[7,8] which is beneficial to lower the manufacturing cost. The enhanced light absorption by SiNW arrays has been demonstrated empirically due to the efficient antireflection to the incident light, especially in the high energy regime of the solar spectrum.[9,10] It is also observed that periodic SiNW arrays are desirable for such a purpose.[11] Recently, the impact of the SiNW length (L) and diameter (D) on the optical characteristics of the SiNW arrays is reported based on a fixed array periodicity (P) of 100 nm.[12] The simulation results show that the excellent light absorption close to 100% is achievable in the high energy region of the solar spectrum ($>\sim 2.8$ eV), in agreement with the experimental results.[9,10] It further indicates that the total solar energy harvesting of the SiNW arrays in the energy region of 1–4 eV, covering the major energy range of the solar spectrum, is lower than that of the Si thin film with the same thickness due to the poor light absorption in the low energy region of the solar spectrum ($<\sim 2$ eV), though it is observed that the light trapping capability can be improved with the SiNW diameter.[12] As will be seen in the following analysis, the overall-inferior light absorption of the above-mentioned SiNW arrays can be attributed to their relatively small feature, i.e., the short periodicity of 100 nm.

In this letter, the impact of the SiNW array P on its optical characteristics is systematically investigated via simulation. Our results indicate that the light absorption can be significantly varied when modifying the array P. It is found that much more efficient light absorption compared to that of the Si thin film with the same thickness can be realized when P is set between 250 and 1200 nm. Further, the ratio of D/P should be >0.5 (or more specifically ~ 0.8) for the optimized solar energy harvesting. The wide window in terms of the SiNW D and array P for improving solar energy harvesting shall facilitate the manufacturing of the highly ordered SiNW arrays for solar cell application. The physics behind the observation is also discussed in this work.

Figure 1 shows the schematic of the SiNW array structure used in this study. The SiNW length is set as 5000 nm, considering the trade-off between the light trapping and the required good standing capability of the SiNW arrays, which is required by the conformal deposition of the transparent electrode on the SiNW surface uniformly for efficient photogenerated carrier extraction along the radial direction. The incident light is in parallel to the SiNW axis, and the energy range of the incident light varies from 1 to 4 eV, corresponding to the wavelength from $\sim$1240 to 310 nm, which covers the major solar spectrum in interest.[13] The simulation is performed using a full wave finite element method.[14] The interaction between the incident light field and the aforementioned structure is realized through infinitely extending the structural unit having the height of 5000 nm and the dimension equal to the SiNW array P, as indicated by the dot line of Fig. 1, in the two-dimensional space by applying the periodic boundary condition. The optical information is thus obtained from the spatial distribution of the energy flux, stemming from the interaction between the incident light and the Si structure.

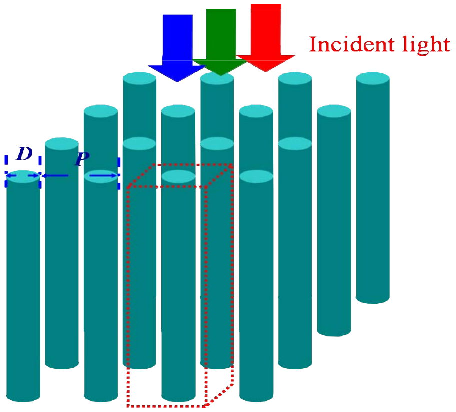

FIG. 1. (Color online) Schematic of the SiNW array structure used in this study. The SiNW length is 5000 nm. The array periodicity and SiNW diameter vary. The incident light is in parallel to the SiNW axis.

---

[a] Electronic mail: hyyu@ntu.edu.sg.

0003-6951/2009/95(24)/243113/3/$25.00

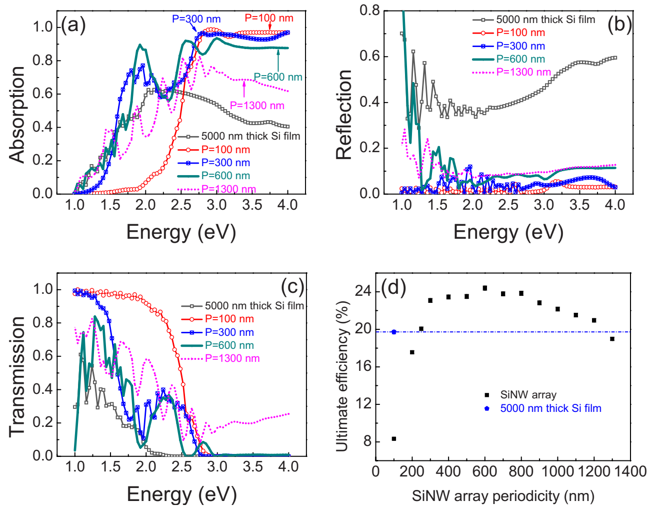

FIG. 2. (Color online) (a) Absorption, (b) reflection, and (c) transmission spectra of the SiNW arrays as a function of P. The ratio of D/P is set as 0.5. The ultimate efficiency is summarized in (d). The 5000 nm thick Si film serves as the reference.

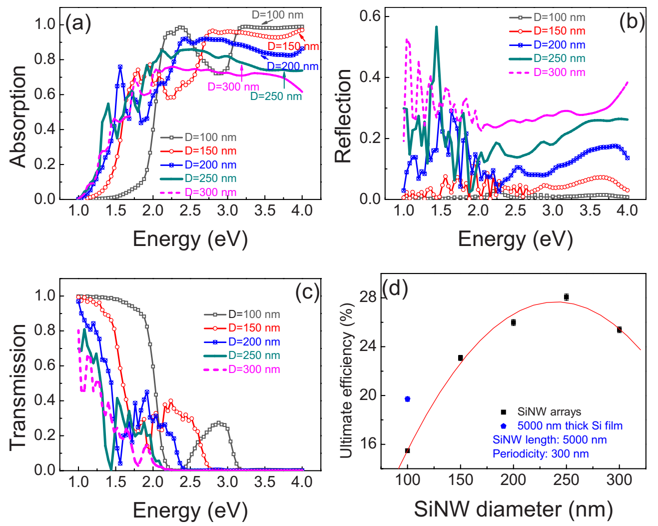

FIG. 3. (Color online) (a) Absorption, (b) reflection, and (c) transmission spectra of the SiNW arrays as a function of D. P is set as 300 nm. The ultimate efficiency is summarized in (d). The 5000 nm thick Si film serves as the reference.

Figures 2(a)–2(c) depict the absorption, reflection, and transmission spectra of the SiNW arrays with different P and the fixed D/P ratio of 0.5. It is obvious that for the SiNW array with a small P, e.g., $\sim$100 nm, the light absorption ($>$95%) mainly occurs in the higher energy regime ($>$2.8 eV), consistent to Hu's observation.[12] With the increase in P, the absorption edge significantly shifts toward the low energy region, which is attributed to the considerable reduction in the light transmission in the low energy region [Fig. 2(c)]. When P is set as 300 nm, higher light absorption than that of the 5000 nm thick Si film is seen for the energy above $\sim$1.6 eV. It is noted that the further increase in P will lead to the decrease in the light absorption in the higher energy region ($>$2.5 eV), which is correlated with the increased light reflection [Fig. 2(b)]. From Figs. 2(b) and 2(c), the light reflection suppression is believed to be the major reason responsible for the improved light absorption observed in all SiNW arrays as compared to the 5000 nm thick Si film.

The aforementioned observations can be explained from the point of view of wave optics.[15] In the low energy region, as the light wavelength is much longer than the SiNW feature, especially for the SiNW arrays with short periodicities, (e.g., when $P=100$ nm), the incident light can thus easily penetrate through the SiNW arrays, resulting in the high light transmission.[15] On the other hand, the wavelength of the incident light in the high energy regime ($>$2.8 eV) becomes comparable with the SiNW feature. For example, the wavelength of the light at 3 eV propagating in the SiNW arrays with the D/P of $\sim$0.5 is $\sim$160 nm based on the effective medium approximation.[16] Accordingly, the scattering effect to the incident light will be dominant, which prolongates the optical path length, and thus significantly boosts the light trapping and suppresses the light transmission.[17,18] With the increase in P, the incident light with the wavelength comparable with the SiNW dimension would shift toward the low energy end, especially for $P<300$ nm, as indicated in Fig. 2(a). Further it should be noted for the large P, e.g., 1300 nm, the separation between neighboring SiNWs would become larger than the incident light wavelength in the high energy regime, leading to the notable light transmission.

Ultimate efficiency (η) is used to evaluate the light absorption capability of the SiNW arrays for solar cell application.[12,15,19] Fig. 2(d) shows the η as a function of P. In agreement with the absorption spectra, η is significantly enhanced and exceeds that of the Si film with the same thickness, i.e., 5000 nm when increasing P from 100 to 250 nm. As P is further increased to $\sim$600 nm, η increases slightly to a maximum value of $\sim$24%, due to the combined effects of the suppressed light transmission in the low energy regime and the increased light reflection. It is noted that when P is $>$600 nm, η decreases slightly due to the light transmission in the high energy regime in addition to the increased light reflection with P.

Figures 3(a)–3(c) show the optical characteristics of the SiNW arrays with different SiNW D at a fixed P of 300 nm. The increase in the SiNW D would also shift the absorption edge toward low energy end and thus facilitate the photon utilization in the low energy regime, which is similar to the case of increasing P (the increase in P shall lead to the D increase due to the fixed D/P ratio of 0.5 as in the analysis of Fig. 2). On the other hand, due to the minimized area between the neighboring SiNWs when increasing D, the light reflection would be increased, and the light transmission would be suppressed. For the case of $D=P$, the properties of the SiNW array become comparable to that of the Si thin film with the same thickness. Accordingly, there also exists a trade-off between the light transmission suppression and the light reflection enhancement with the increase in D for the case of fixed P, which leads to the first increase and then the decrease in η, as shown in Fig. 3(d). It is worth mentioning that this result does not follow the trend reported in Ref. 12, in which η monotonously increases with D, but the value is still lower than that of the Si film with the same thickness as the SiNW arrays.

Figure 4 illustrates the calculated maximum η and the corresponding D/P for the SiNW arrays as a function of P from 300 to 900 nm. It is interesting that for each P, the maximum η can be found when D/P is $\sim$0.8. η of $\sim$30.5% can be realized at the P of 600 nm when D/P is $\sim$0.8.

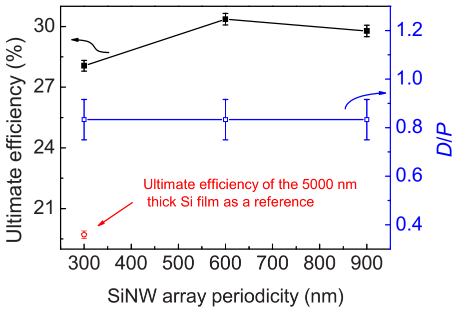

FIG. 4. (Color online) Maximum ultimate efficiency and the corresponding D/P for the SiNW arrays as a function of P from 300 to 900 nm. The ultimate efficiency of the 5000 nm thick Si film serves as the reference.

In conclusion, we have studied the optical characteristics for the SiNW arrays in terms of the array periodicity and SiNW diameter. It was found that the light absorption of the SiNW arrays is sensitive to the array periodicity, and the superior ultimate efficiency than that of the Si film with the same thickness (5000 nm) is achievable for the SiNW arrays when P is set between 250 and 1200 nm. Further, the ratio of D to P should be >0.5 (or more specifically ~ 0.8) for the optimized solar energy harvesting. The wide window in terms of the SiNW D and array P for improving solar energy harvesting shall facilitate the manufacturing of the highly ordered SiNW arrays for solar cell application.

J.L. is very grateful to Dr Y. Li for the technical support and fruitful discussion. Y. H.Y. acknowledges the support from the NTU-NAP (Grant No. M58040005).

[1] K. Peng, Y. Xu, Y. Wu, Y. Yan, S. T. Lee, and J. Zhu, Small **1**, 1062 (2005).
[2] L. Tsakalakos, J. Balch, J. Fronheiser, B. A. Korevaar, O. Sulima, and J. Rand, Appl. Phys. Lett. **91**, 233117 (2007).
[3] E. C. Garnett and P. Yang, J. Am. Chem. Soc. **130**, 9224 (2008).
[4] J. Zhu, Z. Yu, G. F. Burkhard, C. Hsu, S. T. Connor, Y. Xu, Q. Wang, M. McGehee, S. Fan, and Y. Cui, Nano Lett. **9**, 279 (2009).
[5] V. Sivakov, G. Andrä, A. Gawlik, A. Berger, J. Plentz, F. Falk, and S. H. Christiansen, Nano Lett. **9**, 1549 (2009).
[6] M. D. Kelzenberg, D. B. Turner-Evans, B. M. Kayes, M. A. Filler, M. C. Putnam, N. S. Lewis, and H. A. Atwater, Nano Lett. **8**, 710 (2008).
[7] B. M. Kayes, H. A. Atwater, and N. S. Lewis, J. Appl. Phys. **97**, 114302 (2005).
[8] B. Tian, X. Zheng, T. J. Kempa, Y. Fang, N. Yu, G. Yu, J. Huang, and C. M. Lieber, Nature (London) **449**, 885 (2007).
[9] L. Tsakalakos, J. Balch, J. Fronheiser, M. Y. Shih, S. F. LeBoeuf, M. Pietrzykowski, P. J. Codella, B. A. Korevaar, O. Sulima, J. Rand, A. Davuluru, and U. Rapol, J. Nanophoton. **1**, 013552 (2007).
[10] T. Stelzner, M. Pietsch, G. Andrä, F. Falk, E. Ose, and S. Christiansen, Nanotechnology **19**, 295203 (2008).
[11] R. A. Street, P. Qi, R. Lujan, and W. S. Wong, Appl. Phys. Lett. **93**, 163109 (2008).
[12] L. Hu and G. Chen, Nano Lett. **7**, 3249 (2007).
[13] Air Mass 1.5 Spectra, American Society for Testing and Materials, http://rredc.nrel.gov/solar/spectra/am1.5/#1962.
[14] J. Jin, *The Finite Element Method in Electromagnetics*, 2nd ed. (Wiley, New York, 2002).
[15] J. S. Li, H. Y. Yu, S. M. Wong, G. Zhang, X. Sun, G. Q. Lo, and D. L. Kwong, Appl. Phys. Lett. **95**, 033102 (2009).
[16] J. D. Dobrowolski, D. Poitras, P. Ma, H. Vakil, and M. Acree, Appl. Opt. **41**, 3075 (2002).
[17] S. Pillai, K. R. Catchpole, T. Trupke, and M. A. Green, J. Appl. Phys. **101**, 093105 (2007).
[18] S. Koynov, M. S. Brandt, and M. Stutzmann, Appl. Phys. Lett. **88**, 203107 (2006).
[19] W. Shockley and H. J. Queisser, J. Appl. Phys. **32**, 510 (1961).