Optical absorption in c-Si/a-Si:H core/shell nanowire arrays for photovoltaic applications

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The optical properties have been numerically investigated in crystalline Si (c-Si)/hydrogenated amorphous Si (a-Si:H) core/shell nanowire (CSNW) arrays for various structural parameters. We have demonstrated that the light absorption can be greatly enhanced in c-Si/a-Si:H CSNW arrays especially for the weak absorption solar band (1.5–2.5 eV) of crystalline silicon nanowire (c-SiNW) arrays. We have also obtained the optimal parameters for photovoltaic applications, at which the photocurrent enhancement factors have been achieved to be 14% and 345% per volume material compared to in c-SiNW arrays and c-Si films, respectively. Furthermore, the underlying mechanism of the absorption enhancement in CSNW arrays has been discussed. © *2011 American Institute of Physics*. [doi:10.1063/1.3615297]

Crystalline silicon nanowire (c-SiNW) arrays incorporated with the radial p–n junction have great potential for photovoltaic applications.[1] These c-SiNW array solar cells have not only short charge collection lengths due to the radial junction structure, but also strongly enhanced light absorption compared to the bulk counterpart.[2–6] This strong absorption enhancement in c-SiNW arrays, however, rapidly diminishes for the low photon energy (<2.5 eV) due to the indirect bandgap nature of c-Si,[2] which includes the most important solar band (1.5–2.5 eV) of c-Si for photovoltaics.[7] Hence, it may be important to consider additional light trapping that can reinforce the weak absorption in c-SiNW arrays. Such light trapping can be achieved with readily-obtainable core/shell nanowire (CSNW) arrays, consisting of c-Si cores and hydrogenated amorphous Si (a-Si:H) shells, in which the a-Si:H shells may compensate for the weak absorption in c-SiNW arrays since the a-Si:H can be considered to have a direct optical energy gap. In fact, these c-Si/a-Si:H CSNWs have recently been demonstrated to show extremely high light absorption.[8] Nonetheless, the optical properties and their underlying mechanism in such hetero-structured CSNWs have not been much studied to date.

In this Letter, we numerically study the optical properties of c-Si/a-Si:H CSNW arrays, by employing the rigorous coupled-wave analysis (RCWA) method[9,10] that is a frequency-domain simulation to compute electromagnetic diffraction in periodic structures such as c-SiNW arrays.[6] We show that the weak absorption of c-SiNW arrays for the low photon energy (1.5-2.5eV) can be greatly reinforced by coating the a-Si:H shell and also that the absorption of the CSNW arrays can be optimized for photovoltaic applications.

In Figs. 1(a) and 1(b), we show the schematic drawings of c-Si/a-Si:H CSNW square arrays and the top view of an individual CSNW, respectively. CSNW arrays can be characterized by the pitch p, the length L, the core radius r of c-Si, the total radius R (or the a-Si:H thickness $t = R–r$), and the filling ratio f that is defined as $\pi R^2/p^2$. For all the RCWA simulations, we have employed the complex refractive indices of c-Si and a-Si:H taken from Ref. 11, the transverse-electric (TE) and transverse-magnetic (TM) polarized lights at an incident angle of θ with respect to the nano wire (NW) axis in the x–z plane, and the light energy of 1.0–4.0 eV covering the major solar spectrum.

We show absorptance and reflectance as a function of the photon energy in CSNW arrays of $p = 200$ nm, $r = 50$ nm, and $L = 1.0$ μm at $\theta = 0°$ for various a-Si:H thicknesses ($t = 0$–50 nm, corresponding to the filling ratio $f = 0.196$–0.785), in Figs. 2(a) and 2(b), respectively. As shown in Fig. 2(a), the absorption is clearly enhanced for the high photon energy (>2.5 eV) in c-SiNW arrays ($t = 0$) compared to in c-Si films, consistent with the previous results.[2–5] This absorption enhancement may be associated with intrinsically lower reflection in NW arrays than c-Si films, as can be seen in Fig. 2(b). The NW array structure has a large open area, naturally leading to low reflection that perhaps results in high absorption. Also, its comparable dimensions (the NW diameter and the pitch) to the wavelength of incident light renders the optical length prolonged through the interwire light

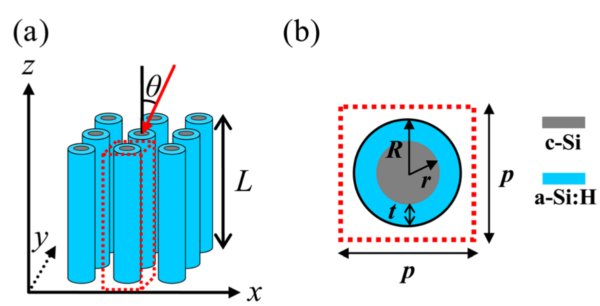

FIG. 1. (Color online) Schematics of (a) c-Si/a-Si:H CSNW arrays of the pitch p and the length L and (b) the top view of an individual CSNW. The red arrow indicates the incident light at an angle θ in the x–z plane.

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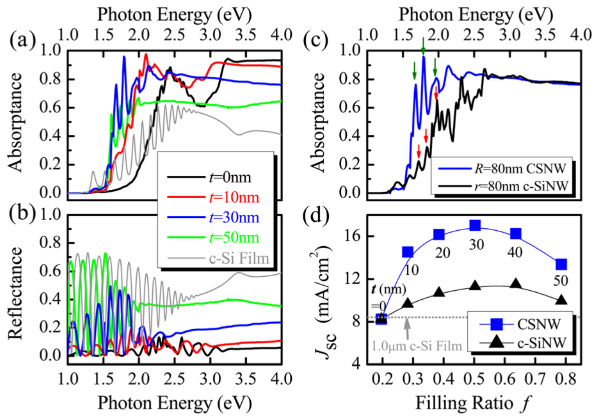

FIG. 2. (Color online) (a) Absorptance and (b) reflectance versus the photon energy in CSNW arrays of $p = 200$ nm, $r = 50$ nm, and $L = 1.0$ μm at $\theta = 0°$ for various a-Si:H thicknesses t. (c) Absorptance versus the photon energy in CSNW arrays of $R = 80$ nm ($t = 30$ nm) and c-SiNW arrays of $r = 80$ nm, both having $p = 200$ nm and $L = 1.0$ μm, at $\theta = 0°$. (d) J_{SC} versus the filling ratio f in CSNW ($r = 50$ nm) and c-SiNW arrays of $p = 200$ nm and $L = 1.0$ μm and c-Si film of 1.0 μm thick.

scattering,[5,12] leading to an effective light trapping. In spite of the strong absorption enhancement for the high photon energy, the absorption in c-SiNW arrays remarkably decreases for the energy range of 1.5–2.5 eV, as shown in Fig. 2(a). This absorption decrease is attributed to the indirect bandgap nature of c-Si that leads to a poor capability to absorb low energy photons (<2.5 eV).[2] Note that although this low energy absorption suppression has been known to be to some extent improved by increasing the NW length, the NW diameter, or/and the pitch, its improvement is rather limited.[2–4] The light absorption in c-SiNW arrays for the low energy (1.5–2.5 eV), however, is greatly boosted by coating a small amount of a-Si:H ($t = 10$ nm), as can be seen in the figure. This absorption enhancement in CSNW arrays can readily be understood by the fact that the imaginary part of complex refractive index that is proportional to the absorption coefficient is ~10 times bigger in a-Si:H than c-Si for the low energy; e.g., it is 0.217 (0.022) for a-Si:H (c-Si) at 2.0 eV.[11] As the shell thickness is increased to 30 nm, the light absorption is further enhanced mainly through distinct absorption resonances. For a further increase of the shell to 50 nm, the intensity of the overall absorption is, however, smaller than that for $t = 30$ nm since a larger material filling ratio for $t = 50$ nm leads to a smaller open area which then results in a larger reflection as can be seen in Fig. 2(b).

Here, we want to discuss the observed absorption resonances that are clearly a major source of the absorption enhancement in CSNW arrays for the low photon energy. In addition to a large open area and the interwire light scattering as mentioned above, there can be another important source of the absorption enhancement due to the leaky-mode resonances (LMRs) in NWs.[13,14] The LMRs, resulting from the interaction between the incident light and the reemitted light in subwavelength structures, have been well-studied in various single NWs.[13–16] These subwavelength resonances are physically different from Fabry-Pérot resonances caused by phase interference between multiple reflections of light. This phase interference effect is typically observed in bulk c-Si films as the gray curve of a regular interference pattern in Fig. 2(a). In our recent work,[16] we have reported a detailed study on the LMRs in both single c-SiNWs and CSNWs, especially showing that the amplified LMRs due to the a-Si shell mainly lead to a significant absorption enhancement in single CSNWs compared to in single c-SiNWs. Also, a recent study has demonstrated that the coupled LMRs can lead the absorption enhancement in bi-SiNWs (i.e., two SiNW system),[17] although there is still a lack of investigation of the LMRs in the NW array system, theoretically and experimentally. Nonetheless, we show absorption resonances occurred in c-SiNW arrays of $r = 80$ nm, some of which are indicated with red arrows in Fig. 2(c). These absorption resonances are clearly enhanced in CSNW arrays of $R = 80$ nm and $t = 30$ nm denoted by green arrows in Fig. 2(c), reminiscent of the amplified LMRs (Ref. 16) and coupled LMRs (Ref. 17). Note that the number of resonance peaks is more in c-SiNW than CSNW arrays, consistent with the result in Ref. 16.

To evaluate the aforementioned absorption enhancement in CSNW arrays for photovoltaic applications, we have calculated the short-circuit photocurrent density J_{SC} as $J_{SC} = \int qF(E)A(E)dE$, where q is the electron charge, $A(E)$ energy-dependent absorptance, and $F(E)$ the spectral photon flux density corresponding to AM 1.5 spectrum.[7] In Fig. 2(d), we present the f-dependent (or t-dependent) J_{SC} for CSNW and c-SiNW arrays of $p = 200$ nm and $L = 1.0$ μm. One can see that J_{SC} for CSNW arrays has the maximum of 17.0 mA/cm^2 at the optimal filling ratio $f = 0.5$ (or $t = 30$ nm) corresponding to the highest light absorption in Fig. 2(a), at which $J_{SC} = 11.3$ mA/cm^2 (8.5 mA/cm^2) for c-SiNW arrays of the same dimensions (c-Si film of 1.0 μm thick). Thus, the photocurrent can be enhanced by ~50% (~100%) in the CSNW arrays of $p = 200$ nm and $L = 1.0$ μm at the optimal filling ratio, as compared to in c-SiNW arrays (c-Si film).

Now, let us vary the pitch p at the optimal filling ratio $f = 0.5$. Figs. 3(a)–3(c) show absorptance, reflectance, and transmittance as a function of the photon energy in CSNW arrays of $f = 0.5$, $r/p = 1/4$, and $L = 1.0$ μm at $\theta = 0°$ for various pitches ($p = 100$–900 nm), respectively. As can be seen in Fig. 3(a), the absorption spectra exhibit a clifflike behavior with high plateaus (60%–87%). Note here that an experimental result also showed high absorption (85%–95%) in similar but disordered CSNWs (Ref. 8), where the even higher plateaus come from the randomness of disordered CSNW system that is known to lead to stronger light scattering than ordered NW system.[5] Nevertheless, the disordered CSNW system does not gain an additional absorption enhancement owing to the absorption resonances, whereas our ordered CSNW system clearly does so as shown in Figs. 2(a), 2(c) and 3(a). For our smallest pitch ($p = 100$ nm), a strong absorption occurs in the high photon energy region (>2.0 eV that is so called the absorption cliff edge). As the pitch is increased to 600 nm, the absorption resonances strongly occur along the cliff hills as in Fig. 3(a), and the absorption cliff edge clearly becomes shifted to the low energy (e.g., the cliff edge is ~1.5 eV for $p = 600$ nm), reminiscent of the diameter-driven red-shift of LMRs (Ref. 14). Note that the NW diameter grows as the pitch is increased for a fixed filling ratio. This diameter-driven absorption edge shift has also been observed in c-SiNW arrays.[3,4] For a further increase of

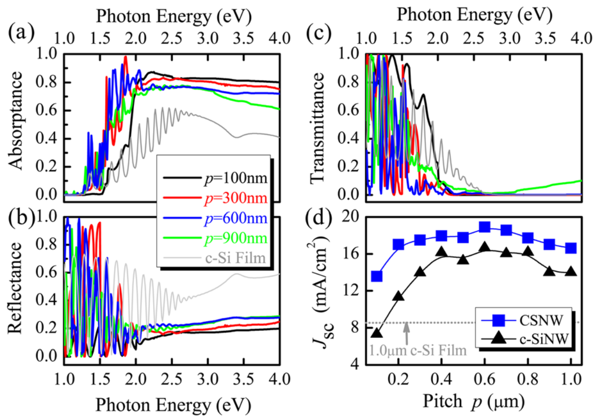

FIG. 3. (Color online) (a) Absorptance, (b) reflectance, and (c) transmittance versus the photon energy in CSNW arrays of $f=0.5$, $r/p=1/4$, and $L=1.0$ μm at $\theta=0°$ for various pitches p. (d) J_{SC} versus the pitch p in CSNW and c-SiNW arrays and c-Si film of 1.0 μm thick.

the pitch to 900 nm, the intensity of the overall absorption (transmission) evidently decreases (increases) compared to the case of $p=600$ nm, due to the less interwire light scattering for the larger dimensions of CSNW arrays. It should also be noted that although the reflection highly depends on the filling ratio as shown in Fig. 2(b), it is insensitive to the pitch of CSNW arrays for the same filling ratio, as can be seen in Fig. 3(b).

In order to obtain the optimal pitch of CSNW arrays for photovoltaic applications, we have calculated the p-dependent J_{SC} in CSNW arrays, as shown in Fig. 3(d), where J_{SC}'s for c-SiNW arrays and 1.0 μm-thick c-Si film are also presented. It is clear from the figure that J_{SC} in CSNW arrays reaches the maximum of 18.9 mA/cm^2 at $p=600$ nm, mainly owing to the absorption enhancement in the low energy. For an increase of the pitch above $p=600$ nm, however, J_{SC} in CSNW arrays slightly decreases due to the overall enhanced transmission above ~1.5 eV, as shown in Fig. 3(c). At $p=600$ nm, on the other hand, $J_{SC}=16.6$ mA/cm^2 (8.5 mA/cm^2) for c-SiNW arrays (c-Si film of 1.0 μm thick). Thus, the photocurrent in c-Si/a-Si:H CSNW arrays can be enhanced by ~14% (~122%) at the optimal pitch, as compared to in c-SiNW arrays (c-Si film). Note here that the practical photocurrent enhancement in CSNW arrays can be ~345% compared to in the c-Si film, if the same volume material is concerned.

With the optimal filling ratio ($f=0.5$) and pitch ($p=600$ nm), we have calculated the L-dependent J_{SC} in CSNW arrays, as shown in Fig. 4(a). J_{SC} is sharply increased as L varies from 0.1 to 5.0 μm and then shows a gradually growing behavior for a further increase of L. Finally, we consider the effect of the incident angle θ of light on the photocurrent or the absorption. In Fig. 4(b), we present the θ-dependent J_{SC} in the 1.0 μm-length CSNW arrays of the optimal configuration ($f=0.5$ and $p=600$ nm) for both the TE and TM polarizations. We also present the J_{SC} for the unpolarized light calculated by averaging those for TE and TM since we only consider the incident light in the x–z plane. Note that the absorption difference between the cases of the incident light in and out-of the x–z plane is known to be negligible.[2] It is very clear that the photocurrent is maintained at a high constant (~20 mA/cm^2) over a large range of the incident angle of light ($\theta=0°$–$70°$), indicating a strongly omnidirectional light absorption in c-Si/a-Si:H CSNW arrays.

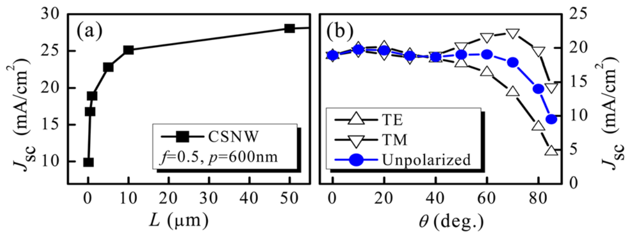

FIG. 4. (Color online) (a) L-dependent J_{SC} in CSNW arrays of $f=0.5$ and $p=600$ nm at $\theta=0°$. (b) θ-dependent J_{SC} in CSNW arrays of $f=0.5$, $p=600$ nm, and $L=1.0$ μm for TE, TM, and the unpolarized light.

In summary, we have performed a numerical simulation study on the optical properties in c-Si/a-Si:H CSNW arrays. We have shown that these heterostructured NW arrays not only retain the superior absorption property of c-SiNW arrays to the bulk counterpart due to their nanostructural benefits, but are able to greatly enhance the weak absorption of c-SiNW arrays, mainly attributed to the absorption resonances. These resonances appear to come from both the amplified (due to the highly absorptive a-Si:H shell) and coupled (due to the array nature) LMRs in the CSNW arrays, however, a further study needs to be performed for clarity. Also, we have found out the optimal parameters to maximize the optical absorption in the CSNW arrays, thus providing a useful developing tool for highly efficient NW photovoltaic devices. Lastly, we want to note that the photogenerated carrier distribution in the CSNW array structure which is of critical importance for designing photovoltaic devices cannot be yielded by the simulation program adopted in this work; however, it has been well-studied in the NW array structure[5] and can be obtained by other simulation methods.[4,18]

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[1] B. M. Kayes *et al.*, J. Appl. Phys. **97**, 114302 (2005).
[2] L. Hu and G. Chen, Nano Lett. **7**, 3249 (2007).
[3] J. S. Li *et al.*, Appl. Phys. Lett. **95**, 243113 (2009).
[4] C. X. Lin and M. L. Povinelli, Opt. Express **17**, 19371 (2009).
[5] H. Bao and X. L. Ruan, Opt. Lett. **35**, 3378 (2010).
[6] W. Q. Xie, J. I. Oh, and W. Z. Shen, Nanotechnology **22**, 065704 (2011).
[7] Air Mass 1.5 Spectra, American Society for Testing and Materials http://rredc.nrel.gov/solar/spectra/am1.5/.
[8] M. M. Adachi *et al.*, Nano Lett. **10**, 4093 (2010).
[9] M. G. Moharam *et al.*, J. Opt. Soc. Am. A **12**, 1068 (1995).
[10] M. G. Moharam *et al.*, J. Opt. Soc. Am. A **12**, 1077 (1995).
[11] E. D. Palik, editor, *Handbook of Optical Constants of Solids* (Academic, New York, 1985).
[12] O. L. Muskens *et al.*, Nano Lett. **8**, 2638 (2008).
[13] L. Y. Cao *et al.*, Nat. Mater. **8**, 643 (2009).
[14] L. Y. Cao *et al.*, Nano Lett. **10**, 439 (2010).
[15] W. F. Liu, J. I. Oh, and W. Z. Shen, IEEE Electron Device Lett. **32**, 45 (2011).
[16] W. F. Liu, J. I. Oh, and W. Z. Shen, Nanotechnology **22**, 125705 (2011).
[17] L. Y. Cao *et al.*, Nano Lett. **11**, 1463 (2011).
[18] S. M. Wong *et al.*, IEEE Electron Device Lett. **31**, 335 (2010).