Light absorption mechanism in single c-Si (core)/a-Si (shell) coaxial nanowires

2011 Nanotechnology 22 125705

(http://iopscience.iop.org/0957-4484/22/12/125705)

IOP PUBLISHING NANOTECHNOLOGY

Nanotechnology **22** (2011) 125705 (4pp) doi:10.1088/0957-4484/22/12/125705

Light absorption mechanism in single c-Si (core)/a-Si (shell) coaxial nanowires

W F Liu[1], **J I Oh**[1,2] **and W Z Shen**[1,3]

[1] Laboratory of Condensed Matter Spectroscopy and Opto-Electronic Physics, and
Key Laboratory of Artificial Structures and Quantum Control (Ministry of Education),
Department of Physics, and Institute of Solar Energy, Shanghai Jiao Tong University,
800 Dong Chuan Road, Shanghai 200240, People's Republic of China
[2] Department of Physics, Boston College, Chestnut Hill, MA 02467, USA

E-mail: wzshen@sjtu.edu.cn

Received 9 December 2010
Published 14 February 2011
Online at stacks.iop.org/Nano/22/125705

Abstract

We have carried out detailed investigations on the light absorption mechanism in single crystalline silicon (c-Si) (core)/amorphous Si (a-Si) (shell) coaxial nanowires (NWs). Based on the Lorenz–Mie light scattering theory, we have found that the light absorption in the coaxial NWs relies on the leaky mode resonances and that the light absorption can be optimized towards photovoltaic applications when the a-Si shell thickness is about twice the c-Si core radius. The photocurrent has been found to be enhanced up to ∼560% compared to c-Si NWs, and to be further enhanced up to ∼60% by coating the nonabsorbing dielectric shells.

(Some figures in this article are in colour only in the electronic version)

Coaxial nanowires (NWs) of crystalline silicon (c-Si or Si hereafter) core and amorphous Si (a-Si) shell have been proposed as one of the promising building blocks for high-efficiency photovoltaic (PV) cells [1–3] as they have the advantage of the long charge carrier diffusion lengths of Si (>200 μm) [4] and at the same time the superior light absorption properties of a-Si [5]. In such Si/a-Si coaxial NW PV cells, the Si core can play a role as an efficient charge collector [6] to compensate for short diffusion lengths of a-Si (∼100 nm) [4], whereas the a-Si shell can be used as an excellent energy absorber to overcome poor light absorption of Si [5], and also as an excellent surface passivator [7]. Recently, single Si/a-Si coaxial NW PVs [1, 2] have been demonstrated to have significantly enhanced photocurrent density (3.5 → 23.9 mA cm^{-2}, i.e. ∼580%) while retaining almost the same open-circuit voltage, compared to Si NW PVs [8]. Also, the light absorption in Si/a-Si coaxial NW arrays has recently been measured to display extremely high absorption rates (85 to 95% at short wavelengths) [3]. Nonetheless, the fundamental mechanism of the light absorption enhancement in Si/a-Si coaxial NWs has never been reported to date.

In this paper, we have employed the Lorenz–Mie light scattering theory [9] to investigate the light absorption in single Si (core)/a-Si (shell) coaxial NWs. We have found not only that our calculated results are in good agreement with the above-mentioned experimental reports [1, 3], but also that the light absorption in the Si/a-Si coaxial NWs is governed by the excitations of leaky mode resonances (LMRs) [10], which is our newly found light absorption mechanism in Si/a-Si coaxial NWs. Also, we have found from this light absorption mechanism that the light absorption can be optimized for PV applications when the thickness of the a-Si shell is about twice the radius of the Si core. In fact, the photocurrent of the Si/a-Si coaxial NWs can be enhanced up to ∼560% compared to Si NWs. In addition, we have also found that a further increase of the photocurrent (up to ∼60%) can be realized by coating nonabsorbing dielectric shells on the Si/a-Si coaxial NWs.

A schematic of the cross section of Si/a-Si coaxial NWs is shown in the inset of figure 1(a). Si/a-Si coaxial NWs can be characterized by the core radius r of Si, the shell thickness t of a-Si, and the total radius $R = r + t$. We have calculated the light absorption in such coaxial NWs within the framework of the Lorenz–Mie light scattering theory, where NWs are treated as infinitely long cylinders, which has been well applied to describing the light scattering and absorption of various single NWs [10–12]. We have employed perpendicular incident light to the NW axis, as indicated by thick arrows in the inset, the wavelength range of 300–1800 nm covering the major solar

---

[3] Author to whom any correspondence should be addressed.

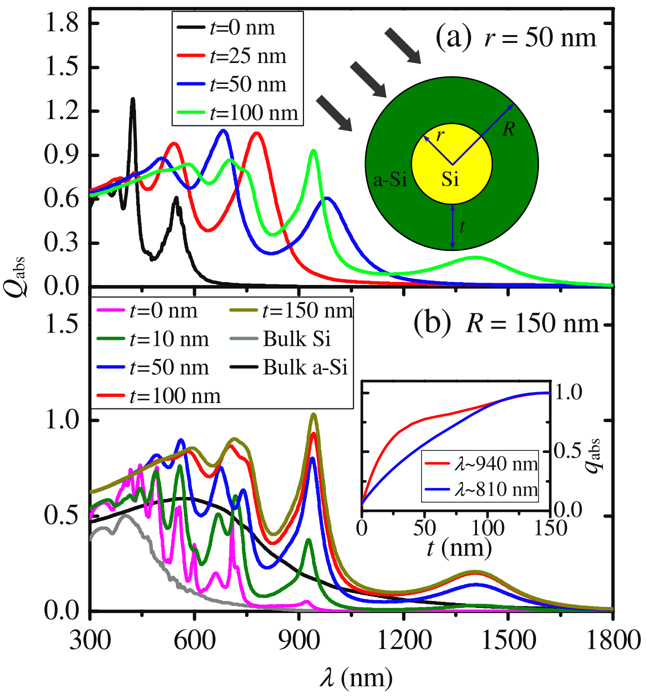

Figure 1. Q_{abs} versus λ in coaxial NWs for various shell thicknesses t at fixed (a) core radius $r = 50$ nm and (b) total radius $R = 150$ nm, together with the bulk Si and the bulk a-Si for comparison. Inset in (a): schematic of the cross section of coaxial NWs with thick arrows representing the incident light. Inset in (b): scaled absorption efficiency q_{abs} versus t at $\lambda \sim 810$ and 940 nm, where $q_{abs} = Q_{abs}(t)/Q_{abs}$ $(t = 150$ nm). Note that Q_{abs} $(t = 150$ nm) is the absorption efficiency in a-Si NWs of radius 150 nm.

spectrum (AM 1.5 G), and the complex refractive indices of Si and a-Si taken from [5]. The absorption efficiency Q_{abs}, defined as the ratio of the absorption cross section to the geometrical cross section of NWs [9], has then been calculated to examine the light absorption capability of the coaxial NWs. For unpolarized sunlight, both $Q_{abs} = (Q_{abs}^{TM} + Q_{abs}^{TE})/2$ and the electric field amplitude E can be readily obtained by solving Maxwell's equations with the boundary conditions at the core/shell and shell/air interfaces [9, 12]. Here, Q_{abs}^{TM} and Q_{abs}^{TE} are the absorption efficiencies for transverse-magnetic (TM, electric field parallel to the axis) and transverse-electric (TE, electric field perpendicular to the axis) illuminations, respectively.

In figure 1(a), we show the wavelength (λ) dependence of Q_{abs} in coaxial NWs of a fixed $r = 50$ nm for $t = 0$, 25, 50, and 100 nm in air. From the figure, one can see clear absorption resonances whose λ-positions and amplitudes exhibit strong dependence on t. Compared to Si NWs ($t = 0$ nm) that have a sharp absorption peak at $\lambda = 423$ nm, the coaxial NWs have a similar light absorption at short wavelengths ($\lambda < 423$ nm), whereas they have greatly enhanced light absorption at long wavelengths ($\lambda > 423$ nm), obviously resulting from a strong light absorption enhancement due to the a-Si shell.

In figure 1(b), we show the Q_{abs} spectra in coaxial NWs of a fixed $R = 150$ nm for $t = 0$, 10, 50, 100, and 150 nm in air, and also show their counterparts in the bulk Si and a-Si. Note that Q_{abs}s of these bulk materials can be readily obtained by considering surface layers of the same thickness as the diameter ($2R$) of coaxial NWs [10]. For increasing t, the number of resonance peaks decreases due to the fact that Si NWs have more resonance peaks than a-Si NWs of the same radius since the imaginary part of the complex refractive index is smaller in Si than a-Si [5]. More importantly, also for increasing t, the light absorption is quickly enhanced, and then becomes saturated for $t > 100$ nm. In fact, as shown in the inset of figure 1(b), in which we present a scaled absorption efficiency $q_{abs} = Q_{abs}(t)/Q_{abs}$ $(t = 150$ nm) as a function of t at two representative wavelengths, i.e. at $\lambda \sim 810$ nm (off-resonance) and $\lambda \sim 940$ nm (resonance), the absorption efficiency of coaxial NWs reaches ~90% of that of a-Si NWs (90.1% for $\lambda \sim 940$ nm and 88.3% for $\lambda \sim 810$ nm) at $t = 100$ nm ($=2r$).

It should be noted here that although there is a slightly higher light absorption for $t > 100$ nm, the performance of those coaxial NW PVs may be degraded due to the poor charge collection of a-Si whose diffusion length is ~100 nm. Thus, the t-dependent light absorption property, i.e. the saturating behavior of the absorption efficiency, may allow us to construct single Si (core)/a-Si (shell) coaxial NW PVs of enhanced light absorption (owing to the a-Si shell) with still high charge collection (owing to the Si core). Moreover, in comparison with the bulk Si and a-Si, the light absorption in the coaxial NWs is significantly enhanced especially at resonance wavelengths, implying that higher photocurrent densities can be induced in the coaxial NWs than their bulk counterparts, which turned out to be so as will be presented later.

The absorption behavior presented above can be understood in terms of the LMRs that may occur in subwavelength structures such as NWs [10, 12] and nanospheres [13]. In NWs, it has been known that the incident light interacts with the re-emitted light, leading to the electric field intensity being resonantly enhanced inside NWs when the wavelength of the incident light matches up with one of the LMRs supported by NWs. The LMRs can be expressed as TM_{ml} or TE_{ml}, where m and l are the azimuthal mode number and the radial order of the resonances, respectively [10]. In figure 2(a), we show the Q_{abs} spectra in coaxial NWs of $r = 50$ nm and $t = 100$ nm under TM (TE) polarized illumination. We also show, in the insets of the figure, the distributions of the electric field intensity $|E|^2$ inside the coaxial NWs at corresponding resonance peaks, designated by arrows. All those resonance peaks can be labeled in terms of the LMRs as TM_{12} and TE_{21} (non-degenerate) near $\lambda = 730$ nm, TM_{21} and TE_{11} (exactly degenerate) at $\lambda = 940$ nm, and TM_{11} and TE_{01} (approximately degenerate) at $\lambda \sim 1400$ nm. This indicates that the absorption resonances in the coaxial NWs originate from the LMRs as in other single NWs [10, 12], due to the nearly identical real parts of the complex refractive indices of Si and a-Si. Also, since the amplitudes of the electric field are clearly stronger in the a-Si shell than the Si core except TE_{11}, the absorption enhancement inside the coaxial NWs arises mainly in the a-Si shell.

In figures 2(b) and (c), we show two-dimensional (2D) Q_{abs}s as a function of R and λ at a fixed $f = t/r = 2$ for TM- and TE-polarized illuminations, respectively. These

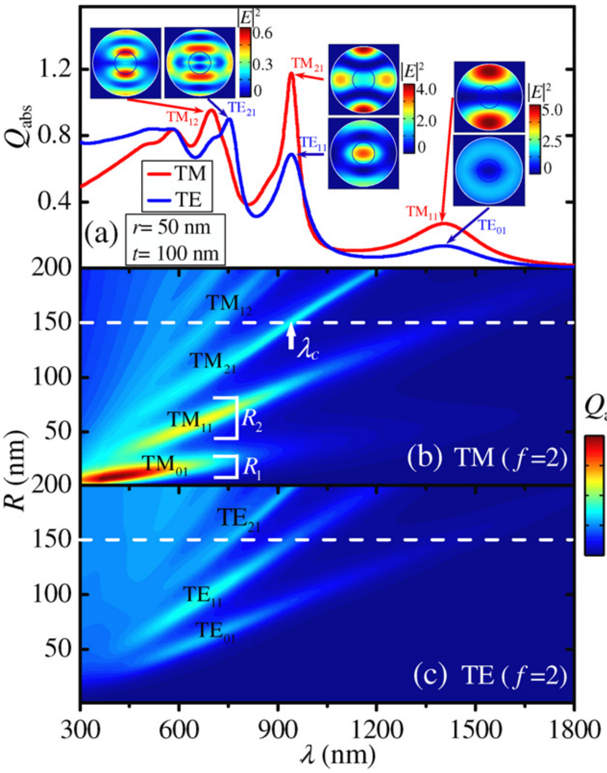

Figure 2. (a) Q_{abs} versus λ for a coaxial NW of $r = 50$ nm and $t = 100$ nm under TM (TE) polarized illumination. Insets: distribution of the electric field intensity $|E|^2$ (normalized to the incident light) inside the coaxial NW for the corresponding peaks indicated by arrows. (b) and (c) 2D Q_{abs}s as a function of R and λ at a fixed $f = 2$ for TM- and TE-polarized illuminations, respectively. The white dashed lines represent the results shown in (a). Important absorption peaks are also labeled with corresponding LMR modes. See text for λ_c, R_1, and R_2.

2D Q_{abs} spectra provide an extensive tunability of the coaxial NW absorption in terms of r, t, and R. The location of each absorption peak can be labeled in terms of the LMRs as shown in the figure, again indicating that the absorption resonances in the coaxial NWs are attributed to the LMRs. Note here that sufficiently small coaxial NWs ($R < 25$ nm) support only the TM$_{01}$ mode but no TE modes, consistent with in other single NWs [10, 12]. Also, at a given R, the coaxial NWs show relatively high absorption at short wavelengths ($\lambda < \lambda_c$), where λ_c depends on R, e.g. $\lambda_c = 940$ nm at $R = 150$ nm as indicated with an arrow in figure 2(b). Such a high absorption behavior at short wavelengths has also been reported in Si (core)/a-Si (shell) coaxial NW arrays [3]. Moreover, it is clear that the light absorption can be optimized when the light absorption spectrum includes the strongest TM$_{01}$ or second strongest TM$_{11}$ mode that corresponds to $5 < R_1 < 25$ nm or $40 < R_2 < 85$ nm, respectively, as indicated in figure 2(b). In fact, we have found that the photocurrent, which is proportional to the light absorption, is strongly enhanced due to TM$_{01}$ or TM$_{11}$ modes, as discussed below.

Now, let us discuss a potential benefit of the coaxial NWs for PV applications. We have calculated the ultimate photocurrent density or short-circuit current density J_{sc} by integrating the product of Q_{abs}, elementary charge q, and the known AM 1.5 G solar flux Γ as $J_{sc}(R, f) = q\int_{300\text{ nm}}^{1800\text{ nm}} Q_{abs}(\lambda, R, f)\Gamma(\lambda)\,d\lambda$. In figure 3(a), we present 2D J_{sc} in coaxial NWs as a function of R and f. As can be seen in the figure, J_{sc} is strongly enhanced with increasing f, and then starts to show a saturating behavior for $f > 2$ (i.e. $t > 2r$), in particular for $R > 50$ nm, to such an extent that $J_{sc}(f = 2) = 93.6\%$ of $J_{sc}(f \to \infty)$ at $R = 150$ nm. In figure 3(b), we show R-dependent J_{sc} in coaxial NWs at a fixed $f = 2$, together with those in Si NWs, and bulk Si and a-Si, having the same volume of materials, for comparison. It is very clear that the coaxial NWs can produce much larger photocurrent than their counterparts. In particular, the coaxial NWs yield $J_{sc} = 28.2$ mA cm^{-2} at $R = 150$ nm (or $r = 50$ nm and $t = 100$ nm), which is a significant enhancement compared to 8.5 mA cm^{-2} in Si NWs. Note here that this calculating result ($J_{sc} = 8.5 \to 28.2$ mA cm^{-2} at $R = 150$ nm) is in good agreement with a recent experimental observation ($J_{sc} = 3.5 \to 23.9$ mA cm^{-2} at a similar size) [1, 2, 8]. It should be also noted that the open-circuit voltage in that experiment was observed not to drop much (0.29 → 0.26 V), implying that Si (core)/a-Si (shell) coaxial NWs can have almost the same electrical properties as Si NWs due to the Si core.

We further show in figure 3(c) the photocurrent enhancement factor (PEF) as a function as R. Here, the PEF is defined as $(I_{sc,cNW}/V_{cNW} - I_{sc,cp}/V_{cp})/(I_{sc,cp}/V_{cp})$, where $I_{sc,cNW}(V_{cNW})$ and $I_{sc,cp}(V_{cp})$ are the photocurrents (volumes) for the coaxial NWs ($f = 2$) and the counterparts (Si NWs, and bulk Si and a-Si), respectively. The PEFs with respect to the bulk materials exhibit a series of local maxima at certain Rs, as indicated with down arrows in figure 3(c), resulting from the effects of the corresponding LMRs, i.e. TM$_{01}$, TM$_{11}$/TE$_{01}$, TM$_{21}$/TE$_{11}$, and TM$_{12}$/TE$_{21}$, from the left to the right. These corresponding PEFs with respect to the bulk Si (a-Si) are 30.1 (4.1), 13.0 (1.7), 8.5 (1.2), and 7.2 (1.0) for $R = 11$, 55, 125, and 165 nm, respectively. Also, the PEF with respect to Si NWs ranges between 2.1 and 5.6 for the entire R investigated.

Finally, we consider the effect of nonabsorbing dielectric shells (only SiO$_2$ in this paper) on J_{sc} in coaxial NWs. In figure 3(d), we show the dielectric shell thickness d dependence of J_{sc} in coaxial NWs for four representative Rs (11, 55, 125, and 165 nm) at a fixed $f = 2$. As clearly seen from the figure, J_{sc}s sharply increase and reach their maxima of 21.8 ($d = 28$ nm), 40.7 ($d = 102$ nm), 46.9 ($d = 134$ nm), and 47.9 mA cm^{-2} ($d = 132$ nm) for $R = 11$, 55, 125, and 165 nm, respectively, indicating that the light absorption and the photocurrent in single Si (core)/a-Si (shell) coaxial NWs can be further enhanced by coating nonabsorbing dielectric shells. These further enhancement factors can be 10, 58, 59, and 61% for $R = 11$, 55, 125, and 165 nm, respectively, by coating SiO$_2$ of the appropriate ds presented above. Note that a thorough analysis of the effect of nonabsorbing dielectric shells on the light absorption in Si NWs can be found in our recent study [12].

In summary, from calculations whose results are consistent with recent experiments [1–3], we have demonstrated that the LMRs play a fundamental role in the light absorption in Si (core)/a-Si (shell) coaxial NWs so that the light absorption can be significantly enhanced by tuning the dimensions of the

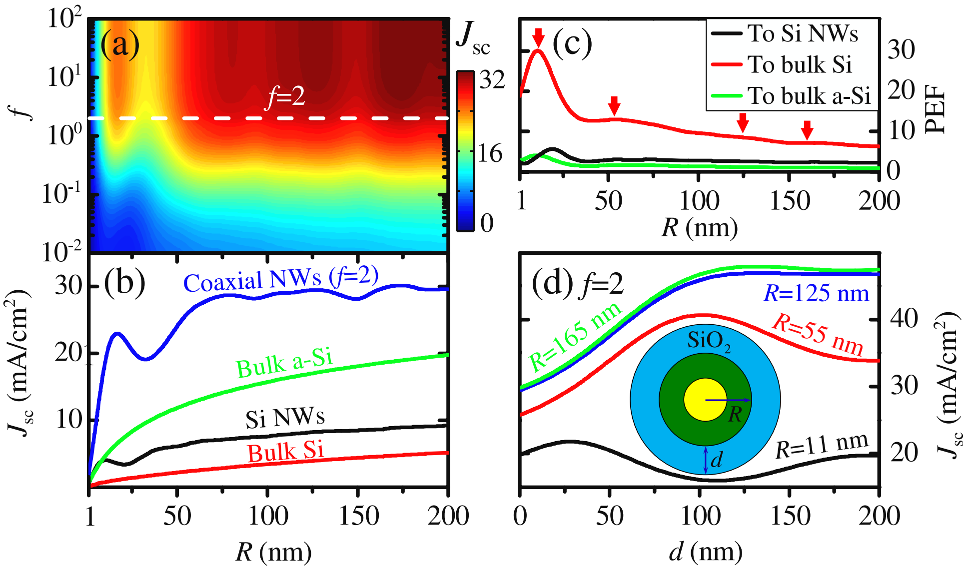

Figure 3. (a) 2D J_{sc} in coaxial NWs as a function of f and R. The white dashed line indicates the case of $f = 2$, replotted in (b). (b) J_{sc} versus R in coaxial NWs for $f = 2$, and in Si NWs, the bulk Si, and the bulk a-Si for comparison. (c) The photocurrent enhancement factors (PEFs) versus R with respect to Si NWs, the bulk Si, and the bulk a-Si. See text for arrows. (d) J_{sc} versus d at $f = 2$ for $R = 11$, 55, 125, and 165 nm. d is the thickness of the nonabsorbing SiO_2 shell. Inset: schematic of the cross section of coaxial NWs with a nonabsorbing SiO_2 shell.

Si core and the a-Si shell while retaining excellent charge carrier pathways. We have also shown that such enhanced light absorption can be further improved by coating nonabsorbing dielectric shells. Therefore, Si (core)/a-Si (inner shell)/SiO_2 (outer shell) coaxial NWs could be a strong candidate for use in constructing high-efficiency NW PV cells.

Acknowledgments

This work was supported by the National Major Basic Research Project of 2010CB933702 and the Natural Science Foundation of China under contracts 10734020 and 11074169.

References

[1] Tian B, Zheng X, Kempa T J, Fang Y, Yu N, Yu G, Huang J and Lieber C M 2007 *Nature* **449** 885
[2] Tian B, Kempa T J and Lieber C M 2009 *Chem. Soc. Rev.* **38** 16
[3] Adachi M M, Anantram M P and Karim K S 2010 *Nano Lett.* **10** 4093
[4] Shah A V, Schade H, Vanecek M, Meier J, Vallat-Sauvain E, Wyrsch N, Kroll U, Droz C and Bailat J 2004 *Prog. Photovolt.* **12** 113
[5] Palik E D 1985 *Handbook of Optical Constants of Solids* (London: Academic)
[6] Dong Y, Yu G, McAlpine M C, Lu W and Lieber C M 2008 *Nano Lett.* **8** 386
[7] Taguchi M, Kawamoto K, Tsuge S, Baba T, Sakata H, Morizane M, Uchihashi K, Nakamura N, Kiyama S and Oota O 2000 *Prog. Photovolt.* **8** 503
[8] Kempa T J, Tian B, Kim D R, Hu J, Zheng X and Lieber C M 2008 *Nano Lett.* **8** 3456
[9] Bohren C F and Huffman D R 1998 *Absorption and Scattering of Light by Small Particles* (New York: Wiley)
[10] Cao L, Fan P, Vasudev A P, White J S, Yu Z, Cai W, Schuller J A, Fan S and Brongersma M L 2010 *Nano Lett.* **10** 439
[11] Cao L, Nabet B and Spanier J E 2006 *Phys. Rev. Lett.* **96** 157402
[12] Liu W F, Oh J I and Shen W Z 2011 *IEEE Electron Device Lett.* **32** 45
[13] Khoury C G, Norton S J and Vo-Dinh T 2010 *Nanotechnology* **21** 315203