Light Trapping in Single Coaxial Nanowires for Photovoltaic Applications

W. F. Liu, J. I. Oh, and W. Z. Shen

***Abstract*—We report a strong enhancement of the light absorption in single coaxial nanowires (NWs) of Si core/dielectric shells. We have calculated the light absorption coefficient within the framework of the Lorenz–Mie light scattering theory and found out that it is greatly increased by effective light trapping in Si cores owing to dielectric shells, as compared to that in Si NWs. We show that the strong absorption of light stems mainly from off-resonance enhancement and also from resonance contribution. By optimally tuning the core radius, the shell thickness, and the shell refractive index, we have obtained ∼102% increase of the photocurrent.**

***Index Terms*—Fano effect, leaky-mode resonances (LMRs), light trapping, off-resonance, single coaxial nanowires.**

I. Introduction

LIGHT trapping is a powerful means to enhance the light absorption of solar cells [1]–[5]. In commercial crystalline Si solar cells, light trapping is typically realized by using the pyramidal textured surface to increase the effective path length of light in the cells [1]. Plasmonics, an emerging field for guiding and localizing light at subwavelength scale, has been becoming a new method for light trapping in thin film solar cells [2]. For nanowire (NW) solar cells, particularly Si NWs with radial p-n junctions [6], although they have been thought to reduce both required quality and quantity of Si due to their intrinsic structure that will orthogonalize the directions of light absorption and charge collection [7], [8], effective light trapping in NW solar cells has not been much studied to date. Recently, there have been some effective light trapping techniques reported in Si microwire *arrays* [3] and in ordered Si NW *arrays* [4]. However, light trapping in *single* NWs still remains unexplored.

It has been shown [5] that one can engineer the resonant property inside *single* NWs by tuning the radius so that the light absorption can be enhanced at resonance regions, so called the leaky-mode resonance (LMR) enhancement [9]. This enhancement effect, however, is rather limited for photovoltaics due to its restriction to resonance regions. On the other hand, the off-resonance absorption enhancement has been known to be more important than the resonance counterpart for photovoltaic applications due to the large wavelength range of the solar spectrum [1]. In this letter, we propose an effective light trapping method in *single* semiconductor NWs by combining both the LMR and the off-resonance absorption enhancements. We have investigated this effective light trapping and corresponding photocurrent enhancement in coaxial NWs that consist of semiconductor NWs such as Si NWs (core) and coated nonabsorbing dielectric materials such as SiO_2, Si_3N_4, and Ta_2O_5 (shell).

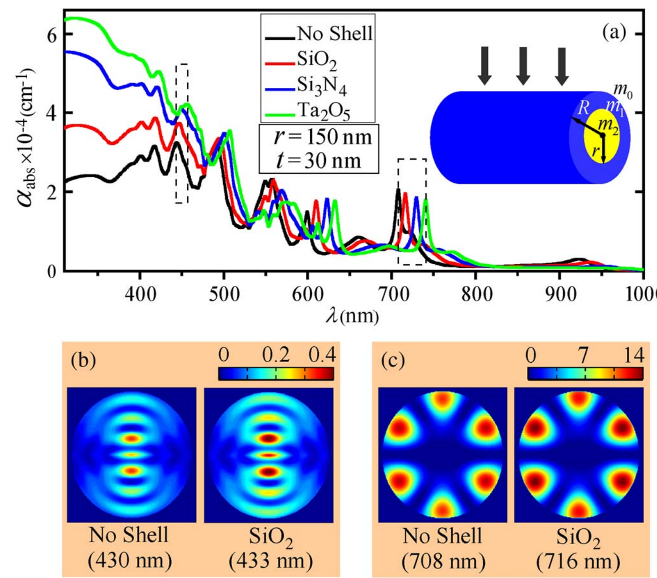

Fig. 1. (a) $\alpha_{\rm abs}$ versus λ. (Inset) Schematic coaxial NW. Yellow (blue) stands for Si core (shell). m_0 (air), m_1 (shell), and m_2 (core) are the refractive indices. Thick arrows indicate incident light. See text for dashed boxes. (b)–(c) Cross-sectional $|E|^2/|E_0|^2$ distributions, shown only inside the core, at (b) off-resonance and (c) on-resonance: (Left) No shell and (right) SiO_2 shell of the same dimension as in (a).

II. Theoretical Method

As in the inset in Fig. 1(a), we have calculated the light absorption of such coaxial NWs in the framework of the Lorenz–Mie light scattering theory [10], where coaxial NWs are treated as infinitely long cylinders, normally illuminated by a plane wave with an incident propagation vector k_0. The cross sections of scattering $(C_{\rm sca})$ and extinction $(C_{\rm ext})$ for transverse-electric (TE, electric field perpendicular to the axis

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of the wire) and transverse-magnetic (TM, electric field parallel to the axis) polarized lights are given by

$$C_{\rm sca}^{\rm TE} = \frac{4}{k_0}\left\{\sum_{n=-\infty}^{\infty}|a_n|^2\right\} \quad C_{\rm sca}^{\rm TM} = \frac{4}{k_0}\left\{\sum_{n=-\infty}^{\infty}|b_n|^2\right\} \qquad (1a)$$

$$C_{\rm ext}^{\rm TE} = \frac{4}{k_0}{\rm Re}\left\{\sum_{n=-\infty}^{\infty}a_n\right\} \quad C_{\rm ext}^{\rm TM} = \frac{4}{k_0}{\rm Re}\left\{\sum_{n=-\infty}^{\infty}b_n\right\} \qquad (1b)$$

where a_n and b_n are far-field scattering coefficients, and the electric field amplitude E inside coaxial NWs can be readily obtained by solving Maxwell's equations with the boundary conditions at the core/shell and shell/air interfaces [10]. If the incident light is unpolarized, like sunlight, we can express the absorption cross section ($C_{\rm abs}$) of coaxial NWs as [10]

$$C_{\rm abs} = \left(C_{\rm ext}^{\rm TE} + C_{\rm ext}^{\rm TM}\right)/2 - \left(C_{\rm sca}^{\rm TE} + C_{\rm sca}^{\rm TM}\right)/2. \qquad (2)$$

Note that the volume absorption coefficient $\alpha_{\rm abs}$, a measure of light absorption ability in coaxial NWs, can be given as $C_{\rm abs}/V_{\rm core}$, where $V_{\rm core}$ is the core volume that is used since the band gaps of the dielectric shells under investigation (310–1100 nm) in this letter are over 4.0 eV ($\sim$310 nm) so that the shells have no contribution to the light absorption. It should be noted that, although the light absorption is usually realized along the axial direction in NW *array* solar cells [3], [4], we consider only the normally incident light in this letter since the light absorption practically occurs along the perpendicular direction in *single* NW photovoltaic devices [5], [7].

III. Results and Discussions

In Fig. 1(a), we show the wavelength (λ) dependence of $\alpha_{\rm abs}$ in coaxial NWs with Si cores of radius $r = 150$ nm and shells of thickness $t = 30$ nm for SiO_2 (refractive index $m_1 = 1.5$), Si_3N_4 ($m_1 = 2.0$), and Ta_2O_5 ($m_1 = 2.3$) in air. Without-shell $\alpha_{\rm abs}$ is shown for comparison. The absorption in the coaxial NWs is clearly enhanced at both resonance and off-resonance regions for short $\lambda < \lambda_c \sim 480$ nm. However, the latter enhancement is twice as much as the former: e.g., 24.6%, 51.7%, or 61.4% at off-resonance ($\lambda \sim 440$ nm) but 14.9%, 27.1%, or 29.5% at resonance ($\lambda \sim 450$ nm) for SiO_2, Si_3N_4, or Ta_2O_5, respectively. In contrast, the light absorption appears to be comparable for long $\lambda > \lambda_c$, resulting in no contribution to the photocurrent enhancement. Note that λ_c is a characteristic wavelength, below which the light absorption enhancement always occurs due to the shells, and can be readily determined for given r, t, and m_1, as found in the inset in Fig. 2(e).

The absorption behavior in Fig. 1(a) can be described in terms of the field distribution inside coaxial NWs. Without loss of generality, due to the similarity of TM and TE spectra [5], we can consider the field (intensity) pattern only for TM. The (normalized) field intensity can be defined as $|E|^2/|E_0|^2$, where E_0 is the incident electric field amplitude. Note that the light absorption in NWs $\alpha_{\rm abs}$ is proportional to the product of the field intensity and the imaginary part of the silicon refractive index that roughly goes as $1/\lambda$ [10]. For $\lambda < \lambda_c$, the field intensity at off-resonance is certainly increased in coaxial NWs with SiO_2, as shown in Fig. 1(b), leading to the strong off-resonance absorption enhancement previously discussed. Note that, for this short-wavelength region, the resonance absorption enhancement in with-shell NWs also results from the increase of the field intensity at resonance, but it is clearly smaller than the off-resonance enhancement previously discussed. For $\lambda > \lambda_c$, although the field intensity of with-SiO_2 NWs is stronger than that of without-shell NWs as shown in Fig. 1(c), the resonance absorption in without-shell NWs is slightly bigger than that in with-shell NWs, as can be seen at $\lambda \sim 710$ nm in Fig. 1(a), since the resonance in without-shell NWs occurs at the smaller wavelength than that in with-shell NWs. Note here that both off-resonance and resonance field intensities of with- and without-shell NWs, as in Fig. 1(b) and (c), show the same patterns that are typical modes inside Si NWs due to the excitation of LMRs [5]. This can allow us to deduce that coaxial NW (with shell) resonances also arise from the excitation of LMRs. As a result, the light absorption in coaxial NWs (with shell) can be enhanced at a desired wavelength by tuning the core radius, likewise in Si NWs.

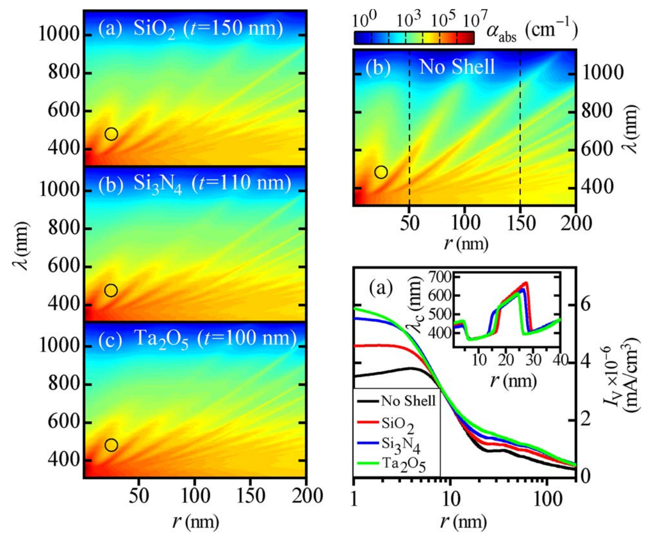

Fig. 2. (a)–(d) $\alpha_{\rm abs}$ versus λ and r. (e) I_V versus r, resulting from (a)–(d). (Inset) λ_c versus r. See text for circles and dashed lines.

The absorption behavior in Fig. 1(a) can be understood by means of the Fano effect [11] that is an interference effect arising from the incident light and the localized reemitted LMR light due to the core of subwavelength size in coaxial NWs. The Fano interference effect is, however, of different origin from that in conventional antireflection coating, where the interference occurs due to the incident light and the phase-shifted reflected light. Recently, the Fano effect has been observed in spherical core/shell nanoparticles [12]. Note that, the lower the field intensity, the weaker the LMRs. For strong LMRs ($\lambda > \lambda_c$), as in Fig. 1(c), such a thin shell ($t = 30$ nm) does not play much role in the light absorption enhancement, since both with- and without-shell absorptions are comparable. However, for weak LMRs ($\lambda < \lambda_c$), as in Fig. 1(b), the incident light ($\lambda \sim 430$ nm) at given subwavelength scales ($r = 150$ nm and $t = 30$ nm) appears to be localized via constructive interference with the reemitted light, resulting in the strong enhancement of the field intensity.

Furthermore, one can see the effects of the refractive index m_1 on the absorption enhancement in coaxial NWs in Fig. 1(a). The light absorption is significantly increased with increasing

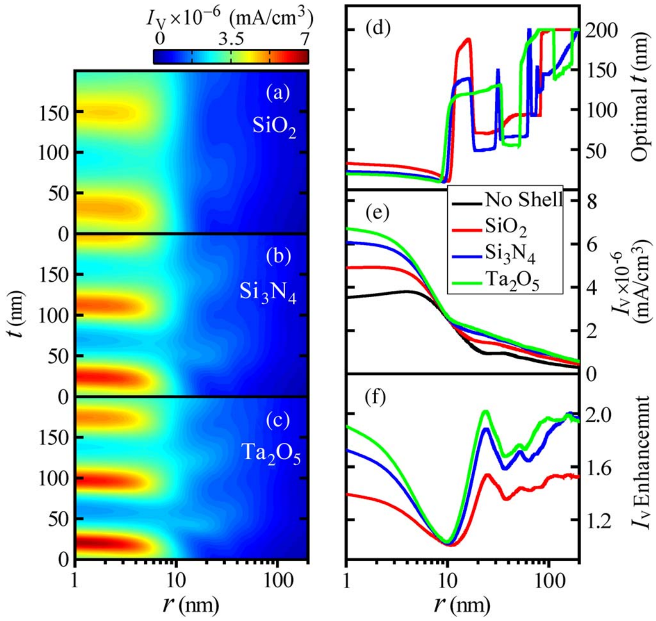

Fig. 3. (a)–(c) I_V versus r and t. (d) Optimal t versus r, resulting from I_V in (a)–(c). (e) I_V versus r, corresponding to optimal t in (d). (f) I_V enhancement versus r, calculated from I_V in (e).

m_1 for $\lambda < \lambda_c$ due to the enhancement of the field intensity inside the Si core with increasing m_1. In addition, the size of m_1-driven red shifts of resonance peaks, as highlighted by the dashed boxes, becomes large with increasing λ, resulting from the increased phase shift of the interference between the incident light and the reemitted light with increasing λ.

Now, we discuss the core size dependence of α_{abs}. In Fig. 2(a)–(c), we present 2-D α_{abs} of coaxial NWs as a function of λ and r for SiO_2 ($t = 150$ nm), Si_3N_4 ($t = 110$ nm), and Ta_2O_5 ($t = 100$ nm), respectively. Note that we used different shell thicknesses, selected from optimal regions that will be clarified later. Fig. 2(d) also shows without-shell α_{abs} for comparison. The absorption in coaxial NWs is clearly enhanced at the off-resonance regions (see circles located at the same spot). Note here that there are common characteristics between with- and without-shell NWs: The number of resonant peaks is augmented with increasing r [see the two dashed lines at 50 and 150 nm in Fig. 2(d)], and these resonant peaks clearly tend to show substantial red shifts with increasing r (r-driven red shift). These common characteristics further imply that the resonance property of coaxial NWs is determined by the core radius.

Under the standard solar spectrum AM1.5G, we can calculate the photocurrent or short-circuit current per unit volume (I_V) as $I_v(r, R) = q \int \Gamma(\lambda)\alpha_{\text{abs}}(\lambda, r, R)d\lambda$, where q is the elementary charge and Γ is the photon flux density, and 100% collection efficiency is assumed to evaluate the ultimate photocurrent. As can be seen in Fig. 2(e), with-shell I_V is certainly increased for the entire region, but $r \sim 10$ nm. The increased amount of I_V, for example, at $r = 24$ nm is 25.7%, 48.4%, or 69.4% for SiO_2, Si_3N_4, or Ta_2O_5, respectively. At $r \sim 10$ nm, the characteristic wavelength λ_c (see inset) is so small ($\lambda_c \sim 370$ nm) that the photocurrent can be hardly enhanced, since the light absorption in the coaxial NWs is mainly enhanced for $\lambda < \lambda_c$, but the solar irradiance is very weak for $\lambda < 370$ nm.

Finally, combining the effects of the thickness of shells (t) with those of the core size (r) and the refractive index of shells (m_1) on the light absorption, we present in Fig. 3(a)–(c) the 2-D I_V in coaxial NWs as a function of r and t for SiO_2, Si_3N_4, and Ta_2O_5, respectively. All the contributions of r, t, and m_1 to the photocurrent I_V fully emerge in these figures: I_V periodically changes in the shell thickness, resulting from the interference behavior of the Fano effect; I_V has maximal values at the small core radius regions, consistent with [5]; and I_V favors dielectric shells of a high refractive index, as previously mentioned. Fig. 3(d) illustrates the optimal t as a function of r, yielded from Fig. (a)–(c). In Fig. 3(e) and (f), we present optimal I_V and its enhancement (the ratio of with- to without-shell I_V) for different r's, corresponding to the optimal t in Fig. 3(d). Except for the weak enhancement of I_V around $r = 10$ nm, as previously discussed, a large I_V enhancement is clearly observed in the coaxial NWs. The maximum enhancement of I_V is 54.1%, 100.1%, or 102.2% for the optimal core/shell NWs of Si ($r = 25$ nm)/SiO_2 ($t =$ 70 nm), Si ($r = 159$ nm)/Si_3N_4 ($t = 180$ nm), or Si ($r =$ 24 nm)/Ta_2O_5 ($t = 124$ nm), respectively.

IV. Conclusion

We have demonstrated an effective light trapping method in single coaxial NWs by coupling the off-resonance enhancement with the LMR enhancement. From the light absorption calculations, we have found that the light absorption in coaxial NWs can be significantly enhanced by tuning their core radius, shell thickness, and refractive index. This strong enhancement readily allowed us to obtain the photocurrent enhancement of up to 102%, implying that this effective light trapping technology can be utilized for high-efficiency NW photovoltaic devices.

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