Light Trapping in Single Coaxial Nanowires for Photovoltaic Applications

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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 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 \(\sim 102\%\) 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 49 nonabsorbing dielectric materials such as SiO\(_2\), Si\(_3\)N\(_4\), and Ta\(_2\)O\(_5\) (shell).

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 \((C_{\text{sc}})\) and extinction \((C_{\text{ext}})\) for 58 transverse-electric (TE, electric field perpendicular to the axis) of coaxial NWs as \([10]\) are given by

\[
\frac{C_{\text{TE}}}{k_0} = \frac{4}{\pi} \sum_{n=-\infty}^{\infty} |b_n|^2 \\
\frac{C_{\text{TM}}}{k_0} = \frac{4}{\pi} \sum_{n=-\infty}^{\infty} |a_n|^2
\]

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 66 absorption cross section \((C_{\text{abs}})\) of coaxial NWs as

\[
C_{\text{abs}} = \frac{C_{\text{TE}} + C_{\text{TM}}}{2} - \frac{C_{\text{TE}} + C_{\text{TM}}}{2}.
\]

Note that the volume absorption coefficient \(\alpha_{\text{abs}}\), a measure of light absorption ability in coaxial NWs, can be given by

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\alpha_{\text{abs}} = \frac{C_{\text{abs}}}{V_{\text{core}}},
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Fig. 1. (a) $\alpha_{\text{abs}}$ versus $\lambda$. (Inset) Schematic coaxial NW. Yellow (blue) stands for Si core (shell), $n_{\text{Si}}$ (air), $n_{\text{Si}}$ (shell), and $n_{\text{Si}}$ (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).

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

**III. RESULTS AND DISCUSSIONS**

In Fig. 1(a), we show the wavelength ($\lambda$) dependence of $\alpha_{\text{abs}}$ in coaxial NWs with Si cores of radius $r = 150$ nm and shells of thickness $t = 30$ nm for SiO$_2$ (refractive index $n_{\text{Si}} = 1.5$), Si$_3$N$_4$ ($m_1 = 2.0$), and Ta$_2$O$_5$ ($m_2 = 2.3$) in air. Without-shell $\alpha_{\text{abs}}$ 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$_3$N$_4$, or Ta$_2$O$_5$, 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 $\lambda_c$ is a characteristic wavelength, below which the light absorption always occurs due to the shells, and can be readily determined for given $r$, $t$, and $m_1$, as found in the inset Fig. 2(e).

The absorption behavior in Fig. 1(a) can be understood by 127 means of the Fano effect [11] that is an interference effect 128 arising from the incident light and the localized reemitted LMR 129 light due to the core of subwavelength size in coaxial NWs. 130 The Fano interference effect is, however, of different origin 131 from that in conventional antireflection coating, where the in- 132 terference occurs due to the incident light and the phase-shifted 133 reflected light. Recently, the Fano effect has been observed 134 in spherical core/shell nanoparticles [12]. Note that, the lower 135 the field intensity, the weaker the LMRs. For strong LMRs 136 in coaxial NWs with SiO$_2$ shell) can be enhanced at a desired wavelength by tuning the 137 core radius, likewise in Si NWs.

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$m_1$ 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 $\lambda$, resulting from the increased phase shift of the interference between the incident light and the reemitted light with increasing $\lambda$.

Now, we discuss the core size dependence of $\alpha_{\text{abs}}$. In Fig. 2(a)–(c), we present 2-D $\alpha_{\text{abs}}$ of coaxial NWs as a function of $\lambda$ and $r$ for SiO$_2$ ($t = 150$ nm), Si$_3$N$_4$ ($t = 110$ nm), and Ta$_2$O$_5$ ($t = 100$ 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 $\alpha_{\text{abs}}$ 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 coaxial 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).

This 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 $\Gamma$ 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$_3$N$_4$, or Ta$_2$O$_5$, respectively. At $r = 10$ nm, the characteristic wavelength $\lambda_c$ (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 ($n_1$) 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$_3$N$_4$, and Ta$_2$O$_5$, respectively. All the contributions of $r$, $t$, and $n_1$ 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 $r$ as a function of $t$, yielded from Fig. (a)–(c). In Fig. 3(e) and 3(f), we present optimal $I_V$ and its enhancement (the ratio of 194 with- and 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$_2$ ($t = 200$ nm), Si ($r = 159$ nm)/Si$_3$N$_4$ ($t = 180$ nm), or Si ($r = 201$ nm)/Ta$_2$O$_5$ ($t = 124$ 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.

### References


