Polymer/Silicon Nanowire Composites for Broadband Absorbance

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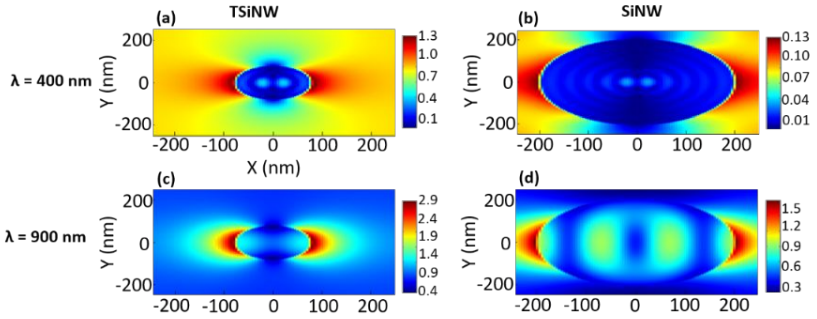

Figure S1: Electric field enhancement around conventional SiNWs (b and d) and TSiNWs (a and c) at 400 and 900 nm, respectively.

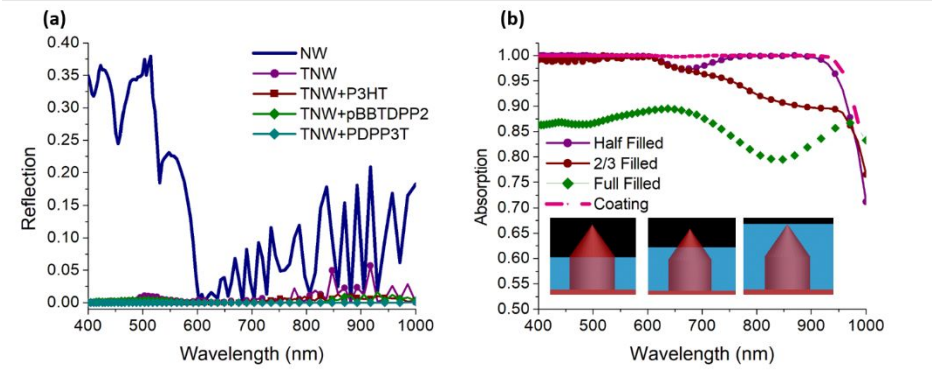

Figure S2: (a) Comparison between the reflection of conventional SiNWs, TSiNWs and TSiNWs coated with different polymers. (b) Absorption simulated for different configurations for the polymer with TSiNWs.

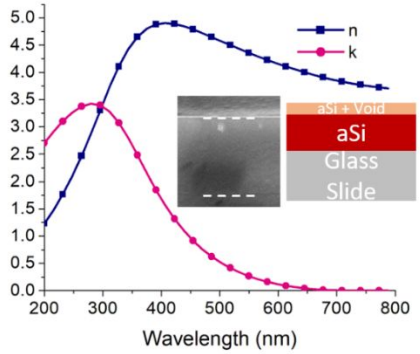

Figure S3: Optical constants of the deposited aSi thin film as determined by the ellipsometry. The inset is the model built in the ellipsometry software.

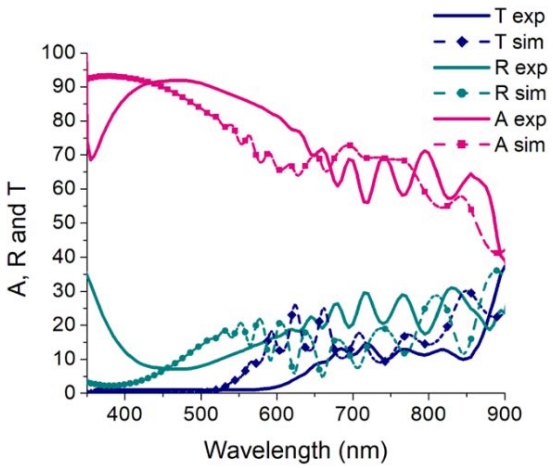

Figure S4: simulated (sim) and measured (exp) absorption of 1.2 μm flat a-Si layer and 200 nm PDPP3T on top.

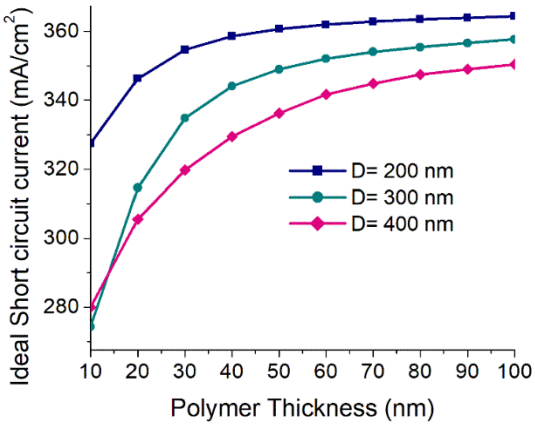

Figure S5: Ideal short circuit current calculated for different polymer coating thickness at different TSiNW diameters.

Modal Analysis

In this section, a 2D modal analysis for the TSiNWs with and without polymer coating is analyzed in different cross sections along the wire to get a full understanding of the optical behavior of the device. Here, the diameter of the NW is 250 nm. The first location used to study is the bottom cylindrical part in the TSiNWs. In this location, the wire is not tapered yet and the modes are identical to the ones of a conventional SiNWs and agree with previously published results[1]. In general, according to previous reports, the two modes propagating in conventional NW are the fundamental mode and a key mode[1,2]. For all wavelengths, the fundamental mode in this location did not change even after the polymer is added as shown in Figure S6(a). The field distribution is confined inside the NW and does not penetrate to the surroundings. This indicates that the coupling of the fundamental mode with the incident light is poor. Thus, this mode does not significantly contribute in the absorption[1].

On the other hand, the key mode shown in Figure S6 (b) at λ= 600 nm is concentrated in the NW and in the air between the NWs. The key modes are the set of strongly absorbing modes, they

couples better to the incident light and they are the ones responsible for the enhanced absorption[2]. It could be seen that adding the polymer caused this mode to be confined in both the NW and the polymer. This indicates that this mode contributes strongly to the absorption. At longer wavelengths (i.e 900 nm), the fundamental mode is the only propagating mode inside the NW[2]. However, it could be seen from Figure S6 (c) that at this wavelength, the mode is poorly confined within the nanowire or the polymer eliminating any resonances and leading to poor absorption.

In the tapered part of the NW, the field distribution starts to change. At 600 nm [Figure S6 (d)], the fundamental mode is still confined inside the NW and the mode confinement does not change after adding the polymer. However, the key mode [Figure S6 (e)] is mainly concentrated in the area between the NWs. After adding the low band gap polymer, mode conferment is found to be stronger in both the NW and the polymer. At λ=900 nm, unlike conventional SiNWs, the fundamental mode is still confined within the NW and the polymer explaining the high absorption calculated at this wavelength.

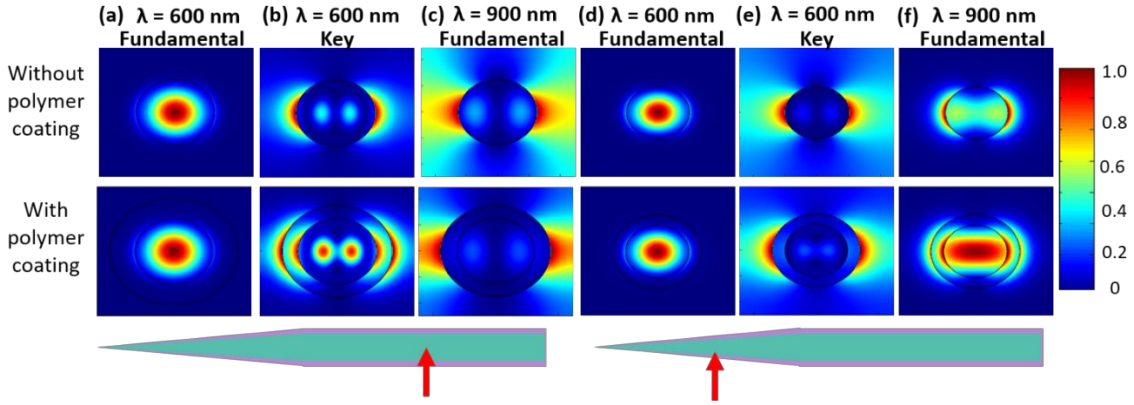

Figure S6: (a,c) The fundamental mode and (b) the key mode with and without polymer coating at multiple wavelengths in the location indicated by the red arrow in the TSiNW underneath. (d,f) The fundamental mode and (e) the key mode in the tapered part of the NW as indicated by the red arrow in the TSiNW underneath.

References

(1) Wang, W.; Li, X.; Wen, L.; Liu, G.; Shi, T.; Duan, H.; Zhou, B.; Li, N.; Zhao, Y.; Zeng, X.; Wang, Y. Optical and Electrical Simulations of Silicon Nanowire Array/Poly(3-Hexylthiophene):Phenyl-C61-Butyric Acid Methyl Ester Hybrid Solar Cell. *Appl. Phys. Lett.* **2014**, *105* (23), 1–6. https://doi.org/10.1063/1.4903872.

(2) Sturmberg, B. C. P.; Dossou, K. B.; Botten, L. C.; Asatryan, A. A.; Poulton, C. G.; de Sterke, C. M.; McPhedran, R. C. Modal Analysis of Enhanced Absorption in Silicon Nanowire Arrays. *Opt. Express* **2011**, *19* (S5), A1067. https://doi.org/10.1364/OE.19.0A1067.