ABSTRACT

Models used in the field of nanoparticle enhanced light-trapping have a wide range of complexity. Often one simply calculates how much power is absorbed in a particular region e.g., a layer of silicon withing a photovoltaic device. It is important to distinguish however “bad” material absorptions from the “good” absorptions which generate current (within a PN junction). Supercomputer simulations can incorporate both the carrier dynamics within a PN junction as well as the optical scattering from nanoparticles but these are too complex for most purposes. We describe herein a new nanophotonic simulation methodology in which we circumvent the complexities of carrier dynamics via an effective loss based on measured responsivity data to model the PN junction. A model for incorporating responsivity in an ad hoc way is shown to yield reasonable results in a low loss limit. We go beyond that limit via another model in which we allow the power we extract from the device to influence the quality of the trap itself.

Keywords: solar energy, photovoltaics, light trapping, nanoparticle scattering.

1 INTRODUCTION

Models used in nanophotonic simulations range from those focused on the macroscopic properties all the way down to those focused on the behavior of a few molecules; and models used in the field of nanoparticle enhanced light-trapping have a similar range of complexity [1-4]. Often one simply calculates how much power is delivered into a particular region. This is important and useful information. To turn this metric into one more germane to the electrical power delivered from a photovoltaic (PV); the responsivity, R (in units of electrical amps output per optical watt input) needs to be incorporated. Additionally, many papers refer to “absorption” and software packages (such as COMSOL which numerically solve the electromagnetic wave equation) can incorporate such as complex permittivity data or as materials models, e.g., the Drude model for free charges and the Lorentz model for bound charges. It’s important to distinguish however that these material absorptions are not the absorptions which generate photo-carrier current (which are characterized by R). This difference is illustrated in Fig. 1, wherein the measurement of an absorption cross-section assesses the optical power transmitted through a sample, in contrast to the measurement of R which assesses the current generated at the PN junction. Recombination increases absorption and Rayleigh scattering dominates the absorption measurement into the UV (as 1/λ^4) but neither of these processes generate relevant photo-carriers in a PV. Thus, those who are utilizing an absorption cross-section might design a trap which has a large improvement factor at say 200nm; but a silicon PV would never yeild that since its responsivity is negligible below 400nm.

Figure1: Schematic of the differences between material absorption and photo-carrier generation.

Simulations on a supercomputer can incorporate the carrier dynamics (within a PN junction) into the optical scattering (from nanoparticles) aspects. But these are time consuming and not generally accessible. We utilize instead: a new nanophotonic simulation methodology in which we circumvent the complexities of carrier dynamics by supplementing existing software packages (which are good at solving the “optics”) with measured responsivity data to model the PN junction. We compare herein, three ways of doing this.

2 AD HOC INCORPORATION OF R

In model A we simply multiply the trapped energy by R (weighted by S(f) the input solar spectrum) and integrate over all frequencies to form an estimate of the short-circuit current J_{sc} via:

\[ J_{sc} = \int d f [S(f) W^R(f) R(f)] \]
where \( W^a = \iint dA \ |E|^2 \) is the electromagnetic energy density integrated over the cross-sectional area of the active region (and we suppressed a units dependent proportionality constant which cancels out in calculating improvement factors). In other words, the appropriate materials models and the trap architectures/dimensions are first chosen. Then the wave equation is numerically solved to determine the electromagnetic field and energy densities that are trapped within the photovoltaic region (e.g., the silicon). It is only after the energy density is calculated that we then weight it by \( R \), in a separate calculation, to form \( f^l_A \). Thus the values of \( R \) in this model do not affect the values of the trapped energy density. Yet, we can think of any light-trap as a resonator – and the improvement factor of the trap as a manifestation of the quality factors (“Q factors”) of the resonator. The Q of a resonator however is perturbed by loss. Thus model A can only hold in the low loss case. This was our first model for incorporating R [1] which has also been recently used by others [2]. To go beyond this (since we want large losses when they are the good ones, i.e., the R-based absorptions) we have devised a model appropriate for the high loss case.

### 3 INCORPORATION OF R AS AN EFFECTIVE LOSS

In model B we allow the amount of power we extract from the device to influence the quality of the trap as follows. From the relation between external quantum efficiency \( \eta \) and \( R \) we obtain a mapping of \( R \) to an effective exponential decay constant times the thickness \( W \) of the material viz.

\[
\alpha W = -\ln(1 - \eta) = -\ln(1 - hf R/q)
\]

which can then be incorporated into existing software packages as if it were an actual material loss, although it is actually an R-based loss. Thus experimentally determined responsivity data can be incorporated in this way (without having to model a PN junction). To model an actual device: \( W \) should be the actual thickness under which the \( R \) curve was measured. To determine the effects of varying the amount of R-based loss however (without altering its spectral dependence) one can simply vary \( W \), as we will do in the following. Using larger \( W \) then will correspond to lowering the overall amount of R-based loss. Therefore

\[
f^B_{sc} = \int \alpha W \sqrt{S(f)} \text{d}f
\]

where, \( W_e = \iint dA \) (Power Absorbed)

and the Power Absorbed is calculated from the numerical solution of the wave equation. We believe this to be the most appropriate model but for the sake of completeness we will also compare to a model C in which we replace equation (4) with \( \iint dA \ |E|^2 \) which is proportional to the electromagnetic energy density integrated over the area of the active region. Figure 2 exemplifies the energy density utilized in model C which is similar to that used in model A (except that the resonant peaks are diminished by the inclusion of the R-based loss).

![Figure 2: Spectrum of \( |E|^2 \) with R-based loss, as used in \( f^C_{sc} \).](image)

Whereas Figure 3 exemplifies the corresponding curve used in model B, which we deem more appropriate since it also incorporates the fact that (here in c-Si) there won’t be any useful absorptions below 400nm. Moreover the spectral shape of \( R \) diminishes the significance of trapped energy peaks that don’t match the peak responsivity of the silicon.

![Figure 3: Spectrum of Power Absorbed, as used in \( f^B_{sc} \).](image)

### 4 COMPARISON OF THE MODELS

We expect that in the low loss limit all three models should yield similar results, i.e., in this limit the ratios of the short-circuit currents should approach a constant (the proportionality constant mentioned above, which in these units is about ten). As the loss is increased however, we would expect a divergence of their predictions so that these ratios would not remain constant as we increase the loss. Figure 4 demonstrates this to be the case. Therein we effectively increase the overall amount of R-based loss when we decrease the \( W \) used in the mapping of equation (2). This
causes both models A and C to underestimate the current generated with respect to our preferred model B. Moreover, in the low loss (large W) limit all three models are seen to yield roughly the same predictions (the ratios converging to the anticipated proportionality constant of about ten).

Figure 4: Ratios of $J_{sc}$ for models A, B and C; for TE and TM polarizations as a function of R-base loss.

REFERENCES


