Light Trapping in Solar Cells Using Nanostructured Reflectors: A Responsivity-Based Model Applied to Waveguide Mode Matching

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ABSTRACT

A responsivity-based model is used to separate the photocarrier generation events ("good absorptions") which generate usefull electricity from the material-based ("bad absorptions") which generate heat. We utilize this to study the attempt to match the spacing of the nanoparticles on the front-scatterer (at a glass/silicon interface) to the parameters of the waveguide modes in the silicon slab waveguide. We find that the perturbation of the waveguide modes by the presence of nanoparticles can prevent such designs from providing resonances at the desired wavelengths. However, if the perturbation is small enough it will primarily only shift the longitunal component of the propagation (k-vector) so that it shifts the resonance peak in a way that can be accurately calculated. This enables a mode-matching design tool which doesn't require extensive calculation of the perturbed modes.

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

1 INTRODUCTION

The global demand for electricity is increasing day by day in an incredible rate. To cope up with this intense thirst of electricity, scientists are coming up with different highly efficient scientific models. Light trapping in solar cells using nanostructured reflectors is one of the promising scientific models which can lead us to an astonishing solution to this problem. Light trapping refers to means by which light not converted to electricity in a single pass through the PN junction of a photodetector or a photovoltaic (PV) is reflected back into the junction. Preferably any such non-converted light is trapped within the device, e.g., by total internal reflection or via some Bragg-type of resonant mode confinement. Many techniques exist and some of the most promising include: the use of plasmonics (arrays of conductive nanoparticles) primarily to generate surface waves to redirect light; the use of photonic crystal (PC) structures typically as back-reflectors; and the use of quantum dots (nanoscale encapsulated semiconductors) which fluoresce and scatter light into different directions.

Simple bandgap models don't accurately match experimentally determined responsivities (R) and many studies focus on material absorption (rather than the photo-carrier events, which are characterized by R). At the other extreme: definitive full-model calculations, including electron/hole dynamics in a PN junction, can take hours to run on a supercomputer. Herein we describe and employ new simulation tools (utilizing experimental R data) which facilitate quick but accurate simulations for understanding and optimization. An expedited simulation methodology is utilized in which the wave equation is solved numerically but electron/hole dynamics in the PN junction are modeled through the use of the experimentally determined responsivity of the unperturbed device.

In our simulations we incorporated the material absorptions utilizing appropriate Drude models since these affect the electromagnetic field distributions of the light-trap and account for the corresponding ohmic losses. We calculated the power delivered to the silicon as a function of wavelength, in db relative to that which would be delivered without any trap and the integral of that power spectral density times the responsivity of the device times the spectral density of the input i.e., Jsc, the short circuit current of the device under such illumination (and concentration via the light-trap). Along with the db-plots we also examined the electric field magnitude distributions for particular wavelengths of interest to understand what works well and what does not.

2 MODELS AND METRICS

We created our models with C-Si and glass slabs in order to turn it into a waveguide supported by the light reflection principles. Models used in nanophotonic simulations range from those designed to analyze macroscopic properties, all the way down to those which focus on the behavior of a few molecules; and models used in the field of light trapping have a similar range of complexity. Definitive fullmodel simulations require a PN junction and a careful incorporation charge carrier dynamics; as well as a good simulation of the optics (scattering at the nanoscale). Many such simulations have been achieved but the computational requirements are more demanding than say the use of software which provides only a good simulation of the optics. Thus, one often simply omits the simulation of a PN junction and models a PV light trap by calculating how much power is trapped into (and absorbed within) a particular region, e.g., a slab of silicon [2]. This is important and useful information. To turn this metric into one more germane to the electrical power delivered from a photodetector, or a PV, a simple bandgap model could be incorporated.

Therein, one assumes the EQE (external quantum efficiency) is a step function in frequency, f ; turning off when the frequency, hence the photon energy, is too low to enable photo-electrons to jump the energy gap into the conduction band. The responsivity, R (in units of electrical amps output, per optical watt input) clearly must be related to the EQE (the number of photo-electrons generated per number of photons absorbed) via R = (q EQE)/(hf) thus, a step in EQE becomes a ramp for R (where h is Planck's constant and q is the charge of the electron). However, such simple bandgap models dont match experimentally measured responsivities; as demonstrated in Fig. 1 wherein we see that the EQE calculated from the measured responsivity of a c-Si PV is not a step function. Thus we like a means of incorporating an experimentally measured R into light-trapping simulations without having to incorporate a PN junction.

Currently, light-trapping simulations which do not incorporate a PN junction utilize material absorption as the basis of their performance metric. Again, this is important and useful information. Its 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 quickly realized by noting that recombination in a real device would increase absorption and Rayleigh scattering dominates absorption into the UV (as $1/_{\lambda^4}$) but neither of these processes generate relevant photo-carriers in a photodetector or PV.

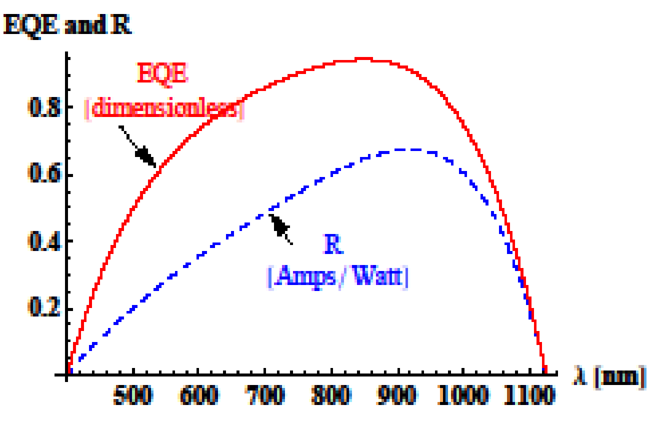

Fig 1: Responsivity of two devices.

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. 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 schematically in Fig. 2 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 (or within the PIN or NIP region, etc.). Recombination increases absorption and Rayleigh scattering dominates the absorption measurement into the UV (as $1/_{\lambda^4}$) but neither of these processes generate relevant photo-carriers in a photodetector or PV.

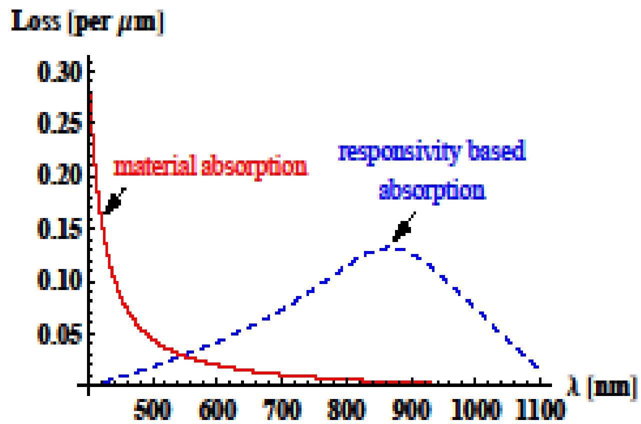

Fig 2: Schematic of the differences between aborption and photo-carrier generation.

3. MODE-MATCHED LIGHT TRAPPING

The silicon PV can function as a dielectric slab waveguide and we can incorporate a perfectly conducting electrode at the bottom of the PV via image theory [2]. Therein we simply use the anti-symmetric modes of a slab twice as thick as our actual one since they will automatically satisfy the boundary condition of zero electric field at the perfect conductor. The modes are set by the simultaneous solution of equations 1 and 2; where from boundary condions we have :

$$Y = -X\,\mathrm{Cot}(X) \qquad \text{(eq.1)}$$

and from $k^2 = k^2_x + k^2_z$ (both inside and outside the slab) which leads to :

$$R^2 = X^2 + Y^2 \qquad \text{(eq.2)}$$

where $X = k_x \frac{d}{2}$ and $R^2 = (n_2{}^2 - n_1{}^2)\left(\frac{\pi d}{1am}\right)^2$

and n_1, n_2 are the indecies of the glass and silicon respectively. To design a mode-matched light trap we can space the nanoparticles (by Lambda) in the front-reflector grating to match the longitudinal periodicity of the guided-mode: Lambda = 2 Pi / k_z = 285.31586537147224 nm for the wavelength for which we want enhanced trapping (we choose 900nm since that is near the peak responsivity). The material properties of silicon are accurately modeled via three Lorentzian terms [3] from which we find n_2 = Sqrt[13.20501118] = 3.6338700004265423 at 900nm. We use this in our initial design and let n_1 = 1.906271229 so that the glass cover can also funtion as an AR coating.

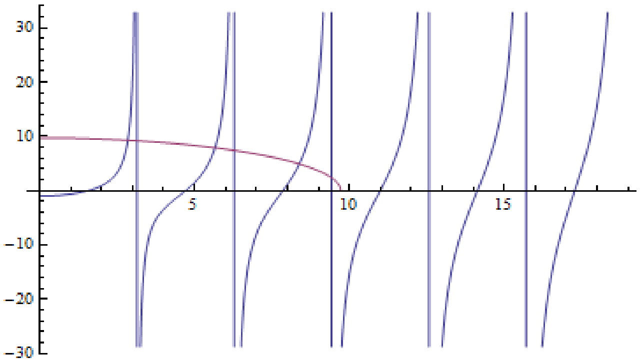

Fig 3: Mode Calculation from the formula.

Fig. 4(a) shows that for d = 400nm we have X from which we calculate k_z = 22.021857421069374 . Indeed, when we have no nano-enhanced trap then the mode pattern in Fig. 4(a) demonstrates "bright spots" (in red) spaced by 142.653 nm as predicted. When we add in nanoparticles the mode pattern is perturbed as shown in Fig.4 (b) and when the size of the nanowires increases we infer that L=(2Pi/k_z)/2 has been changed and we calculate the effective k_x and thereby the new wavelength of the perturbed mode via the simultatneous solution of eq.1 and eq.2. We obtain lam=400-1100nm and indeed Fig. 6(a) shows a strong resonance at that wavelength 567nm (of height = 4.37*10^(-07) units) whereas the initial design wavelength of 900nm only has a ;height = 1.1*10^(-10) units).

For larger perturbations, the effect goes beyond simply shifting k_z. However the above proceedure works for small perturbations and thereby provides a simple design tool for mode-matching in the presence of nanoscattering in those cases.

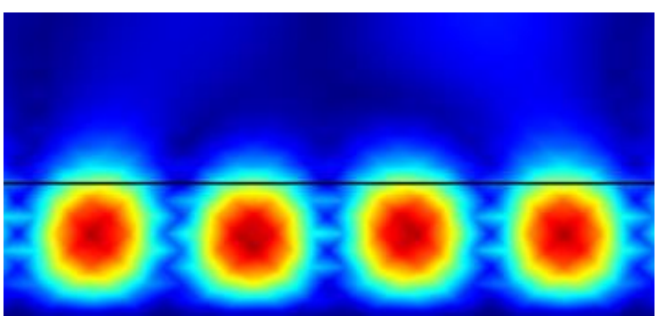
Fig 4(a): Modes created in model having no back reflectors.

We designed the models to get the resonance at 900 nm wavelength. Both Electric and Magnetic field were launched fom the top into the models to find out the efficiency of each model.

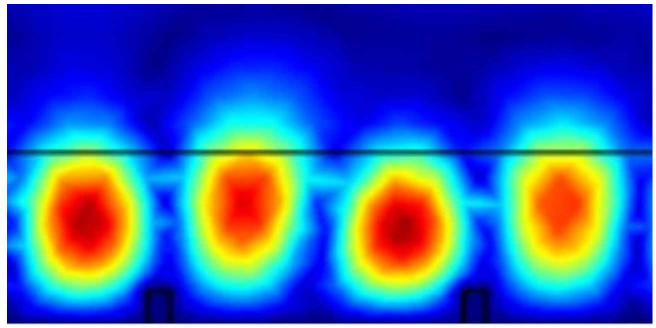
Fig 4(b): Perturbed Modes after using rectangular back reflectors.

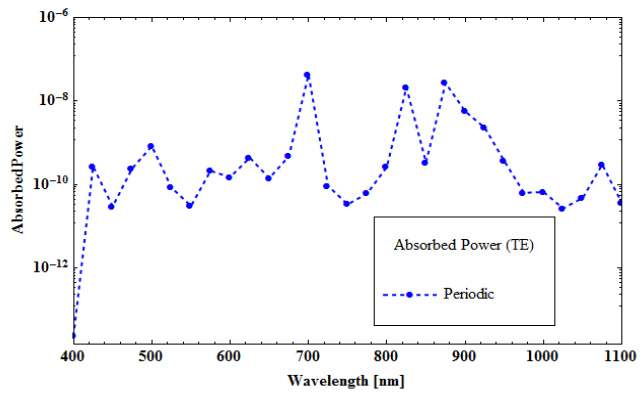

Fig 5(a): Periodic Back Reflector Enhanced model for absorbed power with respect to wavelength at TE Polarization in 25nm Resolution.

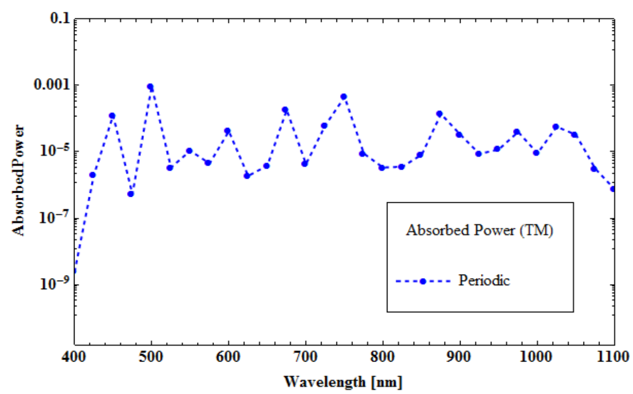

Fig 5(b): Periodic Back Reflector Enhanced model for absorbed power with respect to wavelength at TM Polarization in 25nm Resolution.

We did all the simulations in 25nm resolutions. But from the experience data we saw that the resonance frequency got shifted from 900nm to some other frequency. To find out the the new position of the resonant frequency we launced Electric and Magnetic field into our models from the left end. Due to mode purturbation we got distances between the adjacent modes for specific models at specific wavelenths for side launch. We did the back calculation from this mode perturbation distance to detect the new position of the resonant frequency.

After getting the new position of the resonant frequency we went for higher resolution (1nm) in our simulations to compare the experiment data with the theoritical data. From the experiments we got the highest responsivity points at the theoritically recalculated resonant frequency points.

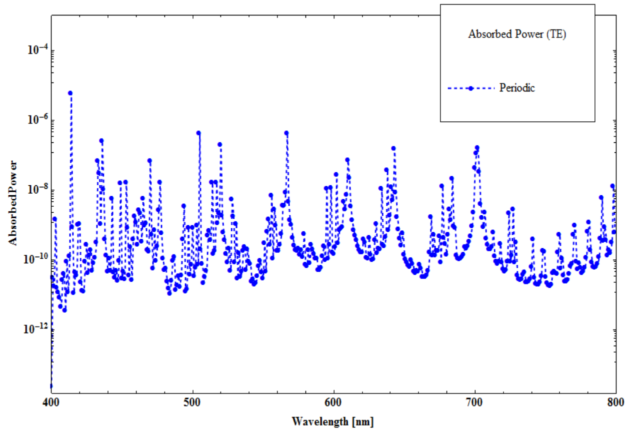

Fig 6(a): Periodic Back Reflector Enhanced model for absorbed power with respect to wavelength at TE Polarization in 1 nm Resolution from 400nm to 799nm.

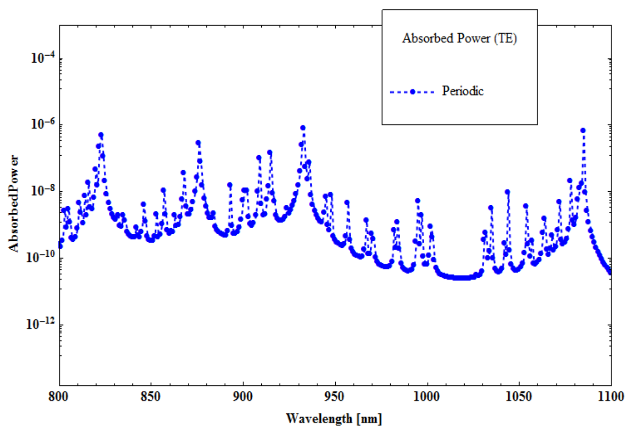

Fig 6(b): Periodic Back Reflector Enhanced model for absorbed power with respect to wavelength at TE Polarization in 1 nm Resolution from 800nm to 1100nm.

We designed our new models with 1nm resolution to get all possible data set in 400nm-1100nm range. From the high resolution data we got to see that the peaks at cetain wavelenghts were even implausibly bigger than they appeared in low resolution simulations.

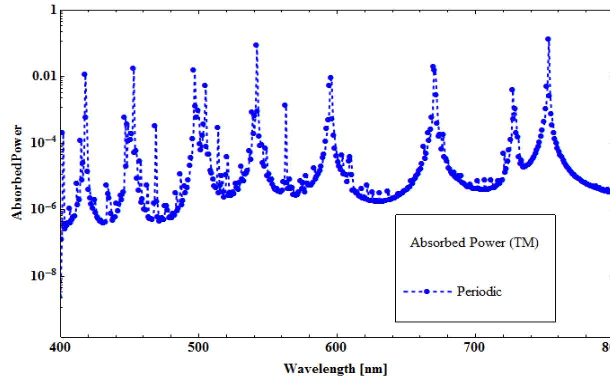

Fig 7(a): Periodic Back Reflector Enhanced model for absorbed power with respect to wavelength at TM Polarization in 1 nm Resolution from 400nm to 799nm.

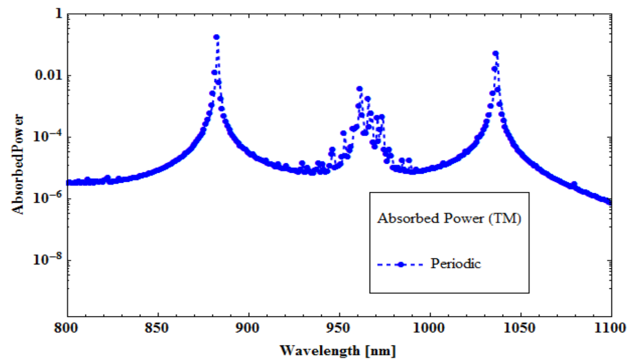

Fig 7(b): Periodic Back Reflector Enhanced model for absorbed power with respect to wavelength at TM Polarization in 1 nm Resolution from 800nm to 1100nm.

CONCLUSION

The best light trapping model can be designed by turning it into a wave guide using the calculated resonant frequency where we can get the highest level of responsivity of particular light polarization. We did the responsivity based waveguide mode maching and came up with the highly efficient model inducing peak responsivity at its resonant wavelengths.

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