Optimization of Nanotoroid Arrays for Plasmonic Solar Cell Applications

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***Abstract*—This work presents the optimization of silver plasmonic nanotoroids in an infinite square array configuration located on top of an amorphous silicon substrate. Using the computational electromagnetics software Ansys® HFSS, the electromagnetic energy absorption enhancement in the silicon layer is optimized by varying the geometric configuration. Percentage enhancement of the generated photocurrent is approximated and is used to compare the performance of various nanotoroid designs, as well as comparison to other geometries.**

I. Introduction

The growing field of nanoplasmonics has illustrated a wide variety of interesting applications, particularly in the field of thin film photovoltaics. Previous works have illustrated that plasmonic nanoparticles located on solar cell surfaces can effectively enhance the electromagnetic energy transmission as well as trap light into lateral modes of the absorbing layer, thereby increasing the energy absorbed and enhancing the generated photocurrent [1-2]. It has been shown that the photocurrent enhancement is highly dependent on the configuration of the nanoparticles, specifically the surface coverage and particle geometry [3-5]. The goal of this work is to perform an investigation of infinite square arrays of nanotoroid plasmonic particles located on a silicon thin-film in order to optimize energy absorption in the silicon layer.

II. Methodology

The commercially available finite element method computational electromagnetics solver Ansys® HFSS is employed to numerically calculate the wavelength dependent plasmonic induced enhancement of electromagnetic fields in a silicon thin-film layer. Fig. 1a illustrates the configuration of the computational domain. This shows a square silicon substrate 500 nm thick in the z-direction with x-y length of $S/2$. (see Fig. 1a). Above the substrate is a 500 nm thick air layer in the computational domain. The nanotoroid is composed of silver and is located 2 nm above the substrate. Boundary conditions as well as toroid geometric parameters R and d are illustrated in Fig. 1b. The simulation is excited by a plane wave propagating in the $-z$ direction with a linear electric field polarization along the x-axis. Due to the symmetry in the excitation and the geometry, prefect **E** and perfect **H** symmetry boundaries are applied to the external y-z and x-z planes respectively. This effectively mirrors the geometry and excitation in two dimensions in the x-y plane and is equivalent to an infinite array of nanotoroids as illustrated in Fig. 1c. S is the center to center spacing between adjacent toroids in the array. Wavelength dependent values of the complex permittivity of silver and silicon are taken from Palik [6]

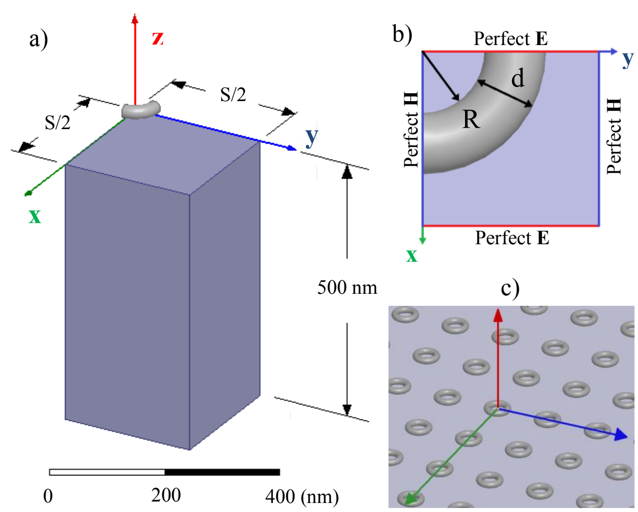

Figure 1. a) Computational setup illustrating quarter toroid located on a 500 nm thick a-Si layer and 500 nm thick air layer on top, b) top view of the domain illustrating the location of perfect **E** and perfect **H** symmetry planes and c) infinite 2D toroid array represented by the computational setup.

In order to evaluate the performance of the nanotoroid arrays a parametric analysis of the design variables R, S and the toroid aspect ratio d/R will be performed. Electromagnetic field enhancement in the silicon layer is quantified by integrating the electric field intensity within the silicon volume. This is used to determine the nanoparticle induced absorption enhancement in the silicon and approximate the generated photocurrent enhancement (PCE), which is integration over all considered wavelengths [7]. By fixing R and d/R the particle spacing S can be parametrically swept to determine the optimal nanoparticle surface coverage.

III. Preliminary Results and Discussion

Fig. 2 shows the preliminary results of the nanotoroid optimization. Here, the average electric field intensity in the silicon layer, $|\mathbf{E}_{Si}|^2_{ave}$ is plotted versus the wavelength for R = 15 nm, d/R = 1 and varying values of the particle spacing S. Although S = 240 nm gives the highest peak $|\mathbf{E}_{Si}|^2_{ave}$ value, the largest photocurrent enhancement occurs at S = 230 nm with 8.2% PCE. This information indicates to possible discrepancy between absorbed fields and the photocurrent enhancement (PCE). However, the PCE metric used here is qualitative and has not been experimentally validated [7]. Additionally, note the local minimum at λ = 855 nm. This reduction of the intensity of the plasmonic resonance at this wavelength indicates that the combination of the interparticle spacing and the incident wavelength are causing slight destructive interference. Because of this dip, the values of $|\mathbf{E}_{Si}|^2_{ave}$ for S = 240 nm between λ = 855 nm and λ = 900 nm are actually lower than the S = 230 nm case. The combination of this and the slight shifting of the resonant wavelength in each of the three cases may explain the reasoning why S = 230 nm provides a slightly higher photocurrent enhancement over S = 240 nm, even though the peak is lower.

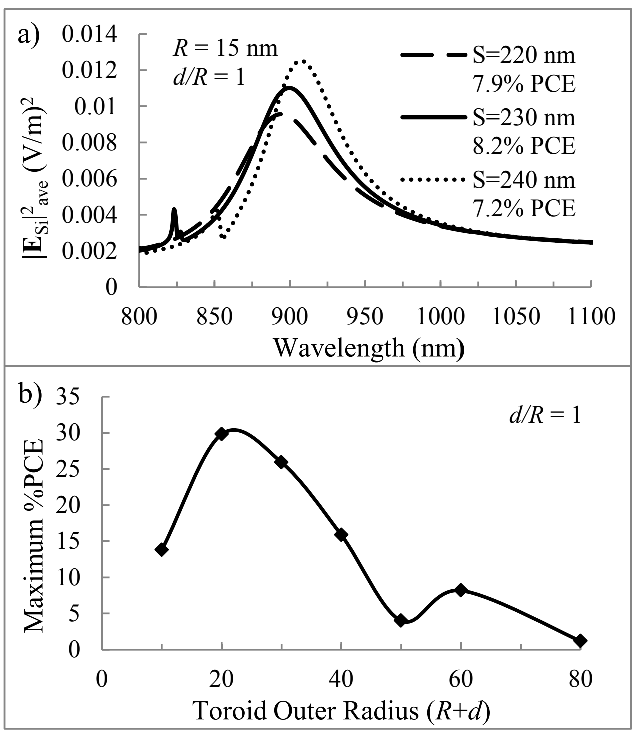

Figure 2. a) Average of the electric field intensity in the silicon layer for silver nanotoroid arrays of R = 60 nm, d/R = 1 and varying particle spacing parameter S. b) Maximum %PCE as a function of nanotoroid outer radius R for the aspect ratio d/R = 1.

The preliminary results of the optimization study are illustrated in Fig. 2b. Here, the maximum %PCE is found by optimizing S for each case and plotted as a function of the toroid outer radius ($R+d$) with all retaining the aspect ratio d/R = 1. The maximum %PCE for all cases occurs at $R+d$ = 20 nm and yields an approximate photocurrent enhancement of 29.8%. These preliminary results are acquired by calculating the field enhancement only for relatively narrow spectral bands covering the resonance location for each case and approximating no effect by the nanotoroids elsewhere.

IV. Conclusions and Future Work

This preliminary work has shown the methods for optimizing plasmonic nanotoroid arrays and illustrates the fact that comparison of maximum resonance peaks is not necessarily a sufficient method for optimization. The results of calculating the %PCE across the entire silicon absorption band from 300 nm to 1100 nm will be presented. In order to determine if optimization over only a narrow band encompassing the nanoparticle resonant frequency, optimization studies using the whole silicon absorbing band will be compared to optimization over a narrower band. Additionally, optimization of silver nanospheres will be performed using this method to provide insight to potential advantages or disadvantages of employing nanotoroid geometry.

Aknowledgement

This work is supported mainly through the NSF/ECCS award # 1006927 and in part through NSF Cyber infrastructure awards EP-0918970 and MRI # 072265 and NSF GK12 award # 0538645. The authors would like to thank the staff of AHPCC for their technical support.

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