Parallel MoM Computation of Localized Field in Silicon due to Finite Array of Nanotoroids

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Abstract: Using nanotoroid antennas on silicon has shown increase in light absorption in photovoltaic (PV) solar cells. The energy efficiency of PVs has shown a potential enhancement as a result of the increase of light absorption. This paper presents computational work to investigate the localized field due to finite nanotoroid arrays on silicon. The absorption increase has been demonstrated in surface current densities on the silicon surface s as well as electric field absorption in silicon. A parallelized version of the method moment surface integral equation is developed for this work. The presented model implements a finite number of nanotoroids versus infinite arrays used in other models. The speed up achieved on large memory nodes is demonstrated. The results show that the field absorption depends on the number of nanotoroids, geometry, and array dimensions.

Keywords: Plasmons, MoM, MPI, Electromagnetic Wave Absorption, Nanoantennas

1. Introduction

Upon illuminating an array of gold or silver nanoparticles with electromagnetic waves at the visible light, they exhibit surface plasmon polariton oscillations at the boundary [1-4]. This phenomenon has been the subject of intensive research to engineer the observed strong localized fields to enhance the efficiency of silicon photovoltaic solar cells [1-2]. Most of published works assumed infinite nanoparticle array, applied the symmetry boundary conditions and computed the field absorption in only one cell which led to significant reduction of the computational burden of the problem [3]. Despite this justifiable assumption, it is necessary to investigate the problem using a finite array and compare the obtained enhancement with those obtained using infinite arrays. The current work considers a finite array of nanotoroids deposited on a finite silicon substrate. The main challenge here is the multiscale nature of the configuration where the silicon surface is much larger than a single nanotoroid. Therefore, the message passing interface (MPI) is implemented to parallelize the conventional three dimensional method of moments surface integral equation model (MoM/SI).

The goal of this work is compare the calculated field absorbed in silicon and to understand the coupling plasmon interactions of nanotoroids with the silicon and with neighboring elements. Nanotoroids are expected to interact directly with each other and/or through surface waves on the silicon/air interface.

2. Methodology

A dimer of nanotoroids immersed in air was investigated using the method of moment (MoM) surface integral equation [4]. The reported results demonstrated a strong increase in localized fields near the dimer surface. In the current work, an array of nanotoroids positioned on silicon is investigated using the MoM. The generated localized fields absorbed in silicon will be calculated to measure the field enhancement which has a potential to increase the efficiency of solar cells. A main challenge here is the need to increase the size of the silicon surface to be much larger the wavelength while the size of each nanotoroid is much smaller the wavelength. As known, the MoM solves a linear system of equations ($ZI=V$), where Z is a full matrix whose size is determined by the number of discretization of silicon surface, the number of nanotoroids in the array, and the frequency. An accurate discretization for modeling this problem generates a matrix that requires large memory and large CPU time to obtain a solution.

A Gaussian beam is used in this work to illuminate the silicon and the nanotoroid array such that the silicon surface edge illumination is minimized upon controlling the beam width [5]. The incident Gaussian beam wave is *y*-polarized with beam width $W=L/6$, where L is the length of the square silicon substrate. In the meantime, the silicon surface size needs to be several wavelengths for all frequencies considered in the band of interest, which is λ=400 nm to λ=1200 nm. To overcome the large memory need, we implemented the standard Message Passing Interface (MPI) parallelization of the MoM computer code [6]. There are other thoughts of accelerators such as the fast multipole method (FMM); however, we first need to investigate some relatively large scale cases before implementing the FMM accelerator even combined with the MPI penalization in the future.

A. MPI Send and Receive commands

To calculate the matrix Z, its elements were divided in a balanced way among all available processors. As known, for large scale matrix Z, the iterative solve is more efficient to use versus matrix inversion. In this work, the Transpose Free Quasi-Minimal Residual (TFQMR) iterative matrix solver was used to solve for the coefficients of surface current densities. A simple pre-conditioner based on the diagonal elements was used to speed up the convergence. To accommodate the necessary communications between all processors involved in the matrix-vector multiplication in the iterative solver, two standard MPI commands were implemented as [6]:

(i) MPI_send (buffer, count, data_type, destination, tag, communicator**)** where buffer is the data to send, count is the number of elements in buffer, data_type is the kind of data types in buffer (i.e. single recession, double precession, integers, real, etc.), destination is the receiver, tag is the label of the message, and communicator is the set of processors involved.

(ii) MPI_recv (buffer, count, data_type, source, tag, communicator, status, error) where source is the sender, tag is the label of message, and status is an integer array with information on message in case of error.

B. MoM Field enhancement factor

Upon calculating the MoM surface current densities, the electric and magnetic fields can be calculated anywhere inside the silicon substrate. In this work, the main interest is the field absorption that occurs at the few micrometers just below the interface. Due to the relatively large wave attenuation in semiconductors, we assumed infinite depth of the silicon substrate and selected the depth of field calculation as needed. The field enhancement factor (EF) is defined as follow [3]:

$$\mathrm{EF} = \frac{\iiint \sigma |\mathbf{E}_{\text{with Nanotoroids}}|^2 dv}{\iiint \sigma |E_{\text{without Nanotoroids}}|^2 dv} \tag{1}$$

where σ the conductivity of silicon. The fields absorbed in silicon will be calculated twice; once with the presence of nanotoroid arrays and once without the array.

3. Numerical Results

Table 1: Wall-time on GORDON HPSC

# Nodes	#CPUs	Wall time (min)
7	112	77.0
12	192	63.5
16	256	62.3
25	400	62.6
40	640	66.06

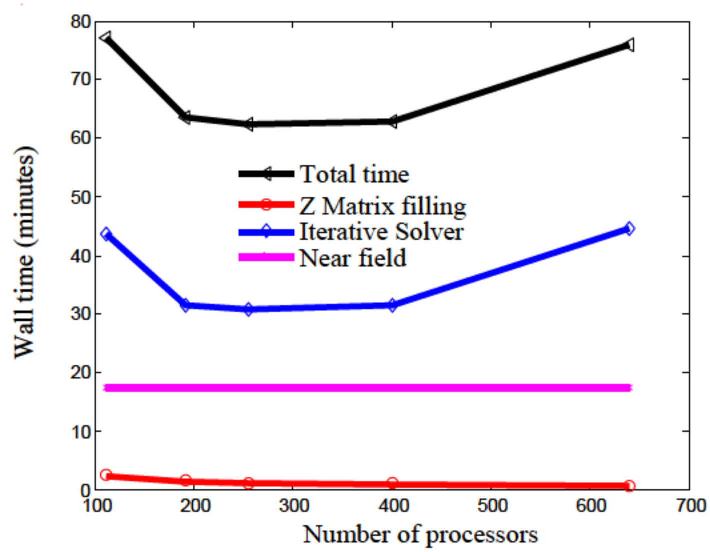

Fig. 1. Wall-time in minutes for the MoM/MPI computer code. All calculations are conducted at single wavelength of 610nm.

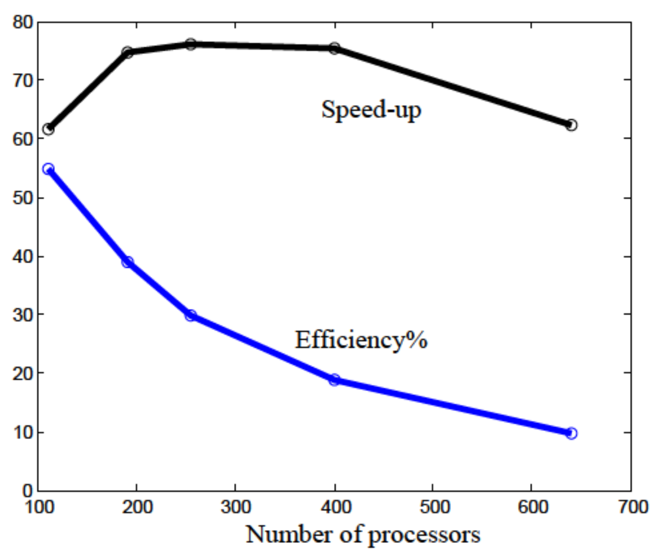

Fig. 2. Speed-up and efficiency of field enhancement computation at wavelength of 610 nm for a 2×1 nanotoroid array of Figure 1.

The nanotoroid arrays are assumed silver in this work and the electrical properties of silver and also silicon are obtained from the literature [7]. Most of the results presented here were obtained using the Gordon supercomputer at San Diego. The size of silicon substrate is assumed 2551nm×2551nm while each nanotoroid has 42nm inner diameter and 84nm outer diameter. Table 1 demonstrates a comparison of the total wall-time on selected GORDON supercomputer nodes. The results are for 2×1 dimer of nanotoroids located on silicon surface where two toroids are located in the *y*-direction and one toroid is located in the *x*-direction with 400 nm separation gap between the centers of nanotoroids.

The GORDON HPSC nodes are Intel EM64T Xeon E5 with 16 cores, clock speed 2.6GHz, flop speed 333 Gflops and memory capacity 64GB and memory bandwidth 85GB. Figure 1 shows the wall-time for each of the parallelized bottleneck of the MoM; the iterative solver including the matrix-vector multiplication, the near field calculations (fields absorbed in silicon), and the filling of matrix *Z*. Figure 2 shows the achieved speed up (running time in serial/running time in parallel) and the efficiency (speed-up/number of processors) of the MoM/MPI computer code, all computed on GORDON.

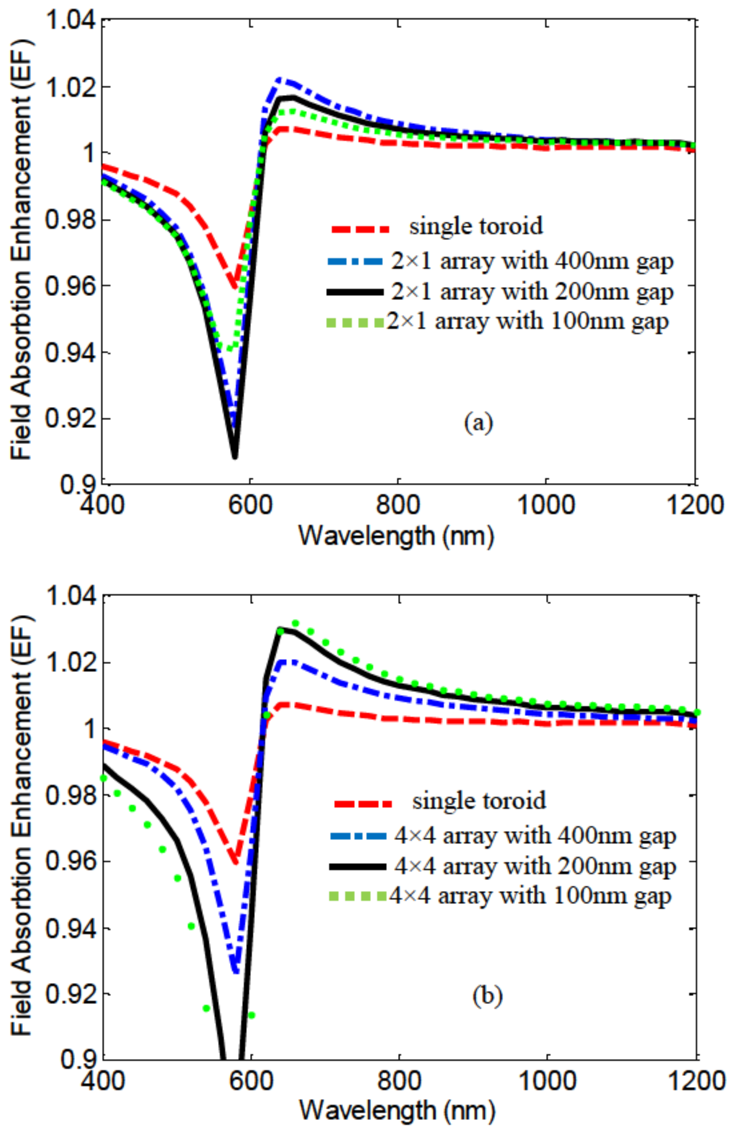

Fig. 3. MoM field enhancement factor (EF) in silicon, due to a (a) 2×1 nanotoroid array and (b) 4×4 array with separation gaps of 400 nm, 200 nm,

As reported in [1-4], the increased absorbed fields in silicon is much localized below the nanotroroids. The obtained results (not shown for limited space) agree with that observation where smaller enhancement was observed when larger surface area was considered in the calculations. The results also demonstrated that the surface current density metric agree in behavior with the absorbed fields; however, the absorbed field calculations take into account the attenuation of surface waves propagating on the silicon interface. As known, the localized fields of nanoparticles are not due to waves propagating in silicon but are due to surface waves [1-4]. On the other hand, the calculation of the fields absorbed in silicon requires increased CPU time as shown in Fig. 1.

The results of Fig. 3 show the field enhancement factor of Eq. (1) for 2×1 and 4×4 arrays with separation gaps 200nm and 400 nm. In all results of Fig. 3, the fields were calculated over a silicon volume of $2W\times2W\times2W$ where $W= L/6$ =417.8nm in this work. The results of Fig. 3 were obtained using 720 processors on GORDON supercomputer (45 nodes). This case required around 48 wall-time hours to calculate the absorbed fields at 41 wavelengths ranging from 400 nm to 1200 nm. The results of Fig. 3a show that the 2×1 array with 400 nm gap demonstrates slightly better enhancement over the array with 200nm gap. The results of Fig. 3b show that the 4×4 array with 200nm gap demonstrates slightly better results than the 400 nm gap, which is the opposite of Fig. 3a. This can be explained by the small size of the silicon surface used in this work. The size of the silicon substrate needs to be several wavelengths in order to obtain accurate results, where in the current work it is only two wavelengths at λ=1200nm.

A. Comparison with the HFSS commercial package

The commercial software Ansys ® HFSS is utilized for comparison of the MoM integral equation results. The geometry consists of a 2×1 nanotoroid array with 200 nm center to center spacing placed 2 nm above the silicon substrate. The silicon is 2551 nm by 2551 nm in the *x*-*y* directions and 850 nm in the *z*-direction, which provides a volumetric geometry closest to one used in the MoM simulation. An infinite array of dimers is assumed on the *x*-*y* plane with 2551 nm spacing between the each toroid dimer pair. Additionally, the geometrical symmetry is exploited to reduce the computational domain to 1/4 of the full domain. Perfect electric conductor boundaries are assumed on the external *x*-*z* planes and perfect magnetic conductor boundaries are assumed on the external *y*-*z* planes which effectively mirror the simulation domain on these planes. The toroids are illuminated here by a plane wave propagating in the –*z* direction versus the Gaussian beam in the MoM case (the incident wave is also linearly polarized in the *y*-direction). The HFSS package is a parallelized one. The results are obtained using the Arkansas High Performance Computing Center using a 256 GB large memory node utilizing 48 processing cores. The domain is decomposed to 327494 tetrahedra where each frequency point requires 2.5 hours of wall time and 94.3 hours of CPU time, indicating a speedup of approximately ×38.

The preliminary results of the HFSS agree in the trend with the MoM results, but the location and the amplitude of the plasmonic peak are not in good agreement between the two methods. The accuracy of the HFSS and the MoM will be increased to obtain better comparison. The comparison results are not shown here for space limit and will be presented in the conference. Also, Gaussian beam excitation will be used in the HFSS to obtain meaningful comparison. Previous work by K. Sendur reported in [8] has illustrated variance in plasmon distribution for sub-wavelength plasmonic nanoparticles illuminated by focused beams of varying beam widths.

4. Conclusions

In this work, the MoM is parallelized using the MPI achieving a speed up of 75 with efficiency 20% on GORDON San Diego Supercomputer. These results show the absorption enhancement in silicon due to nanotoroid array. The preliminary results show small size arrays of max 16 elements. Therefore, the increase shown is not significant (few percentage) where a large volume of silicon was used in the absorption calculations. Results of large array of nanotoroids will be presented in the conference along with a comparison with the HFSS package.

Acknowledgements

This work is supported mainly through the NSF/ECCS award # 1006927 and in part through NSF Cyber infrastructure awards EP-0918970 and MRI # 072265. The computational work was conducted using GORDON San Diego Supercomputer (SDSC). The Authors would like to thank Dr. A. Hassan and the technical staff at the Arkansas High Performance Computing Center and the GORDON supercomputer for their help on the parallelization aspect of this work.

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