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محاسبه توابع گرین فرمولاسیون SIGO با استفاده از روش‌های تسریع همگرایی سری‌ها به منظور تحلیل نانو رزوناتورهای پلاسمونیک

علیرضا قلی پور[۱*] ، فرشته نصراللهی مقدم[۱] و اسفندیار مهرشاهی[۱]

۱- دانشگاه شهید بهشتی، دانشکده برق، تهران، ایران.

a_gholipour@sbu.ac.ir *

چکیده- در تحلیل نانو دایپل‌های پلاسمونیک به روش Surface Impedance Generating Operator (SIGO) نیاز به محاسبه توابع گرین دایادیک است که با حاصل جمع سه گانه بیان شده اند. محاسبه سریع این سری‌ها برای پیاده سازی به روش ممان یک ضرورت است. اما این سری‌ها ذاتا سری‌هایی کند همگرا شونده هستند، خصوصا وقتی که نقاط مشاهده به نقاط منبع نزدیک باشند. در این مقاله سعی می‌شود که تکنیک Ewald که برای تسریع همگرایی چنین سری‌هایی پیشنهاد شده است برای این مساله بهینه شود. این مساله از دو جنبه با مسایلی که قبلا این تکنیک برای آن‌ها بکار گرفته شده متفاوت است. اول این‌که به دلیل نوع خاص فرمولاسیون که برای تحلیل مورد استفاده قرار می‌گیرد، نقاط منبع و مشاهده روی مرز قرار دارند. دیگر این‌که، محیط محفظه که مدلی از بازوهای دایپل پلاسمونیک است، به دلیل ویژگی‌های فلز در فرکانس‌های نوری، به شدت تلفاتی با ضریب شکست منفی است. این خصوصیات لازم می دارد که در اعمال روش‌های تسریع همگرایی متعارف دقت ویژه ای بکار بسته شود. نشان داده خواهد شد که می‌توان با انتخاب مناسب پارامترهای این تکنیک، سرعت بسیار خوبی در محاسبه سری‌ها داشت.

کلید واژه- Surface Impedance Generating Operator (SIGO), Method of Moment (MoM), Plasmonics, Nano-Antenna, Dyadic Green Function.

Calculating Dyadic Green's Function of SIGO Formulation Using Rapid Summation Methods for Analyzing Rectangular Plasmonic Nano-Resonators

Alireza Gholipour[1*], Fereshteh Nasrollahi Moghaddam[1] **and Esfandiar Mehrshahi[1]**

1 Shahid Beheshti University, School of Electrical Engineering, Tehran, Iran.

* a_gholipour@sbu.ac.ir

Abstract- To analyze the nano-dipole antennas using Surface Impedance Generating Operator (SIGO), we need to compute the dyadic Green's functions that are represented in triple summations. For successful implementation of SIGO using the MoM, fast computation of these series is necessary. Unfortunately, these series converge slowly,

especially when the observation points come close to the source points. Ewald sum technique is used to improve the convergence rate of these series. On this paper, we optimize the Ewald method for the problem of plasmonic nano-dipole. This problem differs from those that normally are solved by Ewald sum technique in two main aspects. First, because SIGO is a kind of surface integral equation (SIE) method, both source and observation points are located on the boundary rather than inside the cavity. Second, the materials of nano-dipole arms, which are metals at optical frequencies, are lossy with negative index. These conditions entail that special measures are taken to apply rapid summation techniques effectively. It is shown that by controlling the parameters of rapid summation techniques, good convergence rate is achieved.

Keywords: Surface Impedance Generating Operator (SIGO), Method of Moment (MoM), Plasmonics, Nano-Antenna, Dyadic Green Function.

1. Introduction

Different optical nano structures have been proposed for different applications, including mixers, couplers and sensors in the last few decades. Designing these nano devices requires simulation tools that are able to both effectively model the materials at optical frequencies and also overcome the complexities of nanoscale discretization. Good commercial simulation packages are available for analysing the optical nano devices. However, these packages are not efficient for optimization. Engineering the desired component sometimes needs the optimization process to be repeated thousands of times. If each iteration takes long time to finish, then the optimization will be prohibitive.

Surface integral equation techniques benefit from two advantages compared with other numerical methods in electromagnetics. In contrast to the volumetric methods, the SIE formulations only need to discretise the surface, hence, they have lower number of unknowns. Moreover, the radiation conditions are inherently satisfied by the Green's functions. Therefore, no PML or absorbing boundary condition would be required to terminate the numerical window.

SIGO [1] is a kind of SIE formulation that separates the interior and exterior problems and reduces the main problem into several smaller sub-problems. Each sub-problem can be handled independently. After all, the results are combined to find the solution of the main problem. Due to these specifications, the method is amenable for parallel processing and is efficient for optimization.

In this paper, the analysis of an optical nano dipole using the SIGO formulation is considered. The Green's functions that are needed to be computed for these problems are normally obtained in spectral representation in triple series form [2]. These series converge slowly. So, in order to reach a reasonable precision, one may need to sum many number of terms. Some methods have been proposed to improve the convergence rate of the triple series encountered in rectangular cavities with hard boundary conditions [3]. These methods normally apply the Poisson's formula and introduce the spatial counterpart of the mentioned spectral representation.

A new scheme for very fast computation of the Green's Functions in a rectangular enclosure is introduced in [4], which is based on a Chebyshev polynomial approximation of the vector and scalar potentials in three dimensions. In [5], a new technique is used in which the original spectral series is split into several terms through a Taylor series expansion. Then individual Taylor terms are evaluated. Higher order Taylor terms lead to faster convergence. Finally, Kummer technique is applied to improve the convergence of the remaining series.

The problem of analysing optical nano dipoles using SIGO formulation differs from works with PEC walls in two aspects. First, both source and observation points are located on the boundary. Second, the cavity is made of metals at optical frequencies, which are lossy with negative index. We will show that the proposed Ewald method for

rapid summation can be employed in the current situation, if proper parameters are selected.

The paper is organized as follows. In section 2, formulation of the problem is expressed and in section 3, rapid summation techniques are applied to the dyadic Green's function of optical nano dipole. Some concluding remarks are presented in section 4.

2. Formulation of the Problem

Fig. 1 shows a nono-dipole antenna with two monomers deployed as the arms of the nano dipole, each with volume *V* and surface *S* that is normally made of Au, Al or Ag. Other materials, however, may be used.

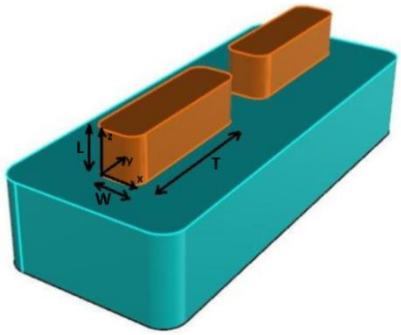

Figure 1 Nano-Dipole Antenna.

In SIGO formulation, an impedance operator is defined as [1]:

$$\mathbf{Z}(\bullet) = j\omega\mu\left[\iint_S \bar{\mathbf{G}}_e^{\text{int}}(\mathbf{r},\mathbf{r}')\cdot(\bullet)ds', \quad \mathbf{r},\mathbf{r}' \in S \right. \qquad (1)$$

Where

$$\nabla\times\nabla\times\bar{\mathbf{G}}_e^{\text{int}}(\boldsymbol{r},\boldsymbol{r}') - \omega^2\mu\varepsilon\bar{\mathbf{G}}_e^{\text{int}}(\boldsymbol{r},\boldsymbol{r}') = \bar{\boldsymbol{I}}\delta(\boldsymbol{r},\boldsymbol{r}')$$

$$\hat{n}\times\left[\nabla\times\bar{\mathbf{G}}_e^{\text{int}}(\boldsymbol{r},\boldsymbol{r}')\right]\Big|_S = \boldsymbol{0} \qquad (2)$$

Generally this dyadic Green function has 9 components [2]. One can use the method of G_A to calculate the required electric dyadic Green function. For the rectangular monomer shown in Fig.1, the vector potential Green function G_A has three diagonal components, each of them is in the following form:

$$G_A^{xx}\left(r,r'\right) = \frac{1}{k^2}\sum_{p=0}^{\infty}\sum_{q=0}^{\infty}\sum_{t=0}^{\infty}\frac{e_p e_q e_i}{TWL\Gamma_{pqi}^2}\sin\left(\frac{p\pi}{w}x\right)\sin\left(\frac{p\pi}{w}x'\right).$$

$$\cos\left(\frac{q\pi}{L}y\right)\cos\left(\frac{q\pi}{L}y'\right)\cos\left(\frac{i\pi}{T}z\right)\cos\left(\frac{i\pi}{T}z'\right) \qquad (3)$$

Where $e_{i,p,q}$ are Neumann coefficients [2] and

$$\Gamma_{pqi}^2 = k^2 - \left(\frac{p\pi}{W}\right)^2 - \left(\frac{q\pi}{L}\right)^2 - \left(\frac{i\pi}{T}\right)^2 \qquad (4)$$

We have to compute the G_A^{xx} in order to be able to represent (1) in matrix form and combine the results with exterior sub-problem.

In equation (3), r and r' are located on the boundary. For the specific component G_A^{xx} the source and observation points are both on the faces parallel to *XY* and *XZ* planes.

In the next section, G_A^{xx} is calculated for different material types and different source-observation point combinations.

3. Rapid Summation Technique

The Ewald sum technique is used to split the dyadic component into two parts. The first part is a hybrid sum of modal series, which is actually a kind of spectral domain representation. The remaining part is introduced in the spatial domain as the image series. These two series are both rapidly convergent, and therefore, the Green's Function can be evaluated correctly with only a few numbers of terms in the series. Utilizing metals with negative index in optical frequencies, leads into imaginary wavenumber (*k*) [6]. Therefore, the parameter Γ defined in (4) will become a complex value having both real and imaginary parts. However, for dielectrics (e.g. glass) the values of Γ are pure imaginary or pure real depending on the mode index. This will affect the convergence rate.

The key component of this technique is a parameter that is called splitting parameter and has a crucial role for the improvement of the convergence rate. This parameter is denoted by *E*. Some suggestions for selecting the value of *E* have been introduced in the literature [7]. In Fig. 2, the effect of *E* values on the convergence of solution

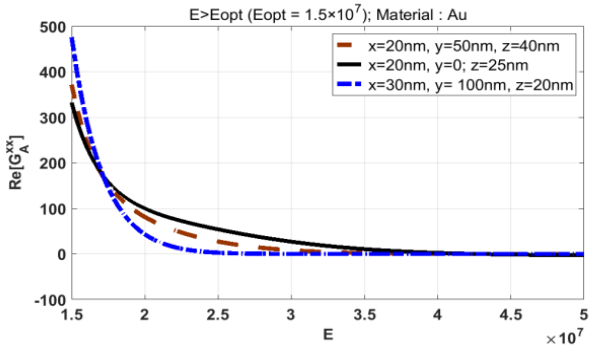

Figure 2 Convergence of G_A^{xx} as *E* changes.

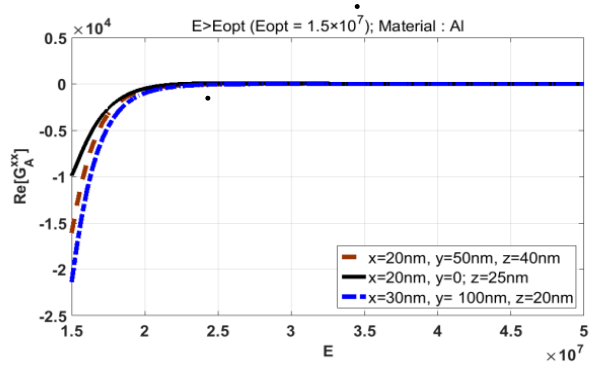

Figure 3 Convergence of G_A^{xx} as *E* changes.

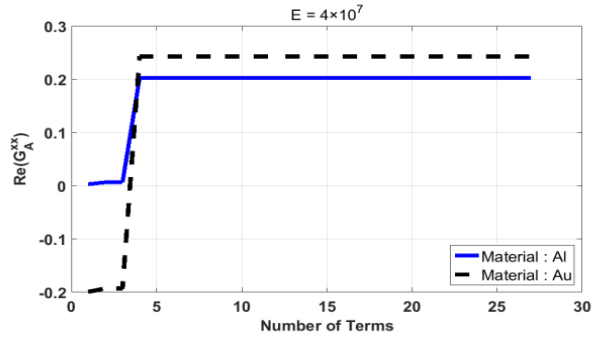

Figure 4 Number of terms needed in Ewald technique.

can be observed. The number of terms for spectral part is selected to be 6 (Fig. 4). This convergence can be obtained by direct summation, when at least about 27000 numbers of terms are summed together. This takes around 5.5 seconds which is almost 500 times more than the required time for Ewald sum technique. Therefore, considerably faster computation is achieved. In all presented results, the source point is located at *x'=20nm* , *y'=0* , *z'=20nm*. Different observation points as well as material types are considered. It is worth mentioning that Eq (3) and consequently the presented results are valid for all rectangular monomers that are depicted in Fig. 1. For other geometries, the required Green's Dyads should be computed in advance.

As shown in Figures (2) and (3), when the observation point is far from the source, the convergence occurs faster than the time it is placed in a closer distance.

4. Conclusion

The Ewald sum technique was applied to the electric dyadic Green's function of SIGO formula. It was shown that proper value of splitting parameter would lead to successful summation and rapid convergence when the metals at optical frequencies are analysed.

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