Simulation of Infinite Nano-array using the Periodic Volume Integral Equation Method

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Abstract—**This paper presents an effective electromagnetic analysis method for simulating infinite nanoarray. Instead of the infinite nanoarray, only a unit needs to be calculated by the Volume Integral Equation (VIE) Method with the periodic Green's functions (PGF). A numerical result validates the accuracy and efficiency of the method.**

Keywords—the Volume Integral Equation; periodic Green's functions; nanoarray

I. INTRODUCTION

Progress in the field of nanotechnology has greatly propelled the experimental investigation and exploitation of novel effects at the nanoscale. Due to the unique features of plasmons, such as the tunable resonance and the near-field enhancement, it has wide applications in biosensing, clean energy, and spectroscopy. However, in the exploratory stage, experimental methods may result in a large number of resource consumption. Therefore, electromagnetic simulation is an effective method to research the nanoarray and more environmental friendly.

In this paper, the Volume Integral Equation (VIE) Method with the periodic Green's functions (PGF) is used to simulate infinite nanoarray by analyzing a unit of the structure. The Volume Integral Equation can be used to fit the shape of the unit structure and describe the material properties. Therefore, the simulation of the infinite nanoarray can be simplified to analysis a single nano particle, which greatly reduces the calculation domain and saves the computing resources. The Volume Integral Equation with the periodic Green's functions can provide effective theoretical reference for the design of nanoarray. At the same time, the experiment cost is saved effectively.

II. FORMULATIONS

Assume a plane wave is incident on the continuous periodic structure under polar and azimuthal angles (θ,ϕ). The periodic structure extends to infinity in two directions, which can be divided into infinite number of identical basic units, as is shown in Fig. 1. $A=|\mathbf{a}\times\mathbf{b}|$ is the surface of the primitive cell, and $\mathbf{k}_{mn}=m\mathbf{k}_1+n\mathbf{k}_2$ is the translation vector.

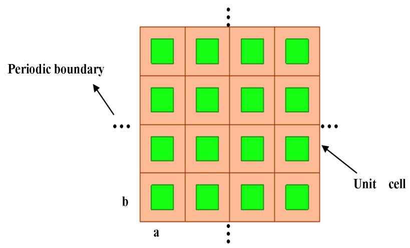


Fig.1. Geometry of a periodic structure

According to the boundary condition that tangential current of perfect conductor surface is zero, the Volume Integral Equation (VIE) can be obtained as follow

$$\mathbf{E}^{inc}=\mathbf{D}/\hat{\varepsilon}+j\omega\mathbf{A}+\nabla\Phi_V \tag{1}$$

where

$$\mathbf{A}(\mathbf{r})=\frac{\mu}{4\pi}\int_V \mathbf{J}(\mathbf{r})G_0 d\mathbf{r} \tag{2}$$

$$\Phi_V(\mathbf{r})=\frac{1}{4\pi\varepsilon}\int_V \rho(\mathbf{r})G_0 d\mathbf{r} \tag{3}$$

and V is the basic unit area, $\mathbf{D}(\mathbf{r})$ is the electric current density on a single basic unit, and $\mathbf{G}_0(\mathbf{r},\mathbf{r}')$ is the periodic Green's function.

The representation of the 2D periodic Green's functions (PGF) is given [2] by

$$G_0=\sum_{m=-\infty,n=-\infty}^{\infty}\frac{e^{-jk_0 R_{mn}}}{4\pi R_{mn}}e^{j(k_x^i ma+k_y^i nb)} \tag{4}$$

and

$$R_{mn}=\sqrt{(x-x'+ma)^2+(y-y'+nb)^2+(z-z')^2} \tag{5}$$

corresponds to the distance between the observation point at (x,y,z) and the source in the unit cell of the infinite array.

To solve the electric field integral equation, the SWG basis function is used to discrete the electric current density. And we use Galerkin method to test the whole electric field integral equation. Taking the inner product of this the electric field integral equation can be obtained as follow

$$\left\langle \mathbf{E}^{inc}, \mathbf{f}_m \right\rangle = \left\langle \mathbf{D} / \hat{\varepsilon}, \mathbf{f}_m \right\rangle + j\omega \left\langle \mathbf{A}, \mathbf{f}_m \right\rangle + \left\langle \nabla \Phi_V, \mathbf{f}_m \right\rangle \tag{6}$$

By the above formula，which leads to

$$\begin{aligned}\int_V \mathbf{f_m} \cdot \mathbf{E}^{inc} d\mathbf{r} &= \int_{V_m} \mathbf{f_m} \cdot \frac{\mathbf{D(r)}}{\hat{\varepsilon}(r)} d\mathbf{r} + j\omega \int_{V_m} \mathbf{f_m} \cdot \mathbf{A}(\mathbf{r}') d\mathbf{r} \\ &- \int_{\Omega_m} (\nabla \cdot \mathbf{f_m}) \Phi_V(\mathbf{r}') d\mathbf{r} + \int_{V_m} (\mathbf{n} \cdot \mathbf{f_m}) \Phi_V(\mathbf{r}') d\mathbf{r}\end{aligned} \tag{7}$$

where Ω_m is the boundary surface and $\mathbf{n}$ is the normal component of Ω_m. And then we can obtain the matrix equation that we want to solve

$$\left[Z_{mn} \right] \left[D_n \right] = \left[v_m \right] \tag{8}$$

where the right side of the vector is v_m , Z_{mn} is the impedance matrix, D_n is the dielectric current coefficient, which is the unknown quantity that we want.

III. NUMERICAL RESULTS

The example simulates the thin-film nanoarray. Fig. 2 illustrates the schematic pattern of the Ag cube. The scale of the unit cell is $2nm \times 2nm \times 2nm$ and the periodic of nanoarray is $8nm \times 8nm$, and the unknown is 242. The scattered electric field $\left| E^{sca} \right|$ is calculated with the proposed method. A normal incidence plane-wave illuminated on the structure at a frequency of 375THz. Fig. 3(a) and Fig. 3(b) show the simulation result of Near-field distribution in the section profile by FEKO and VIE individually.

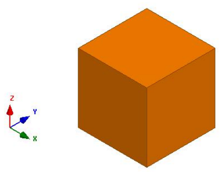
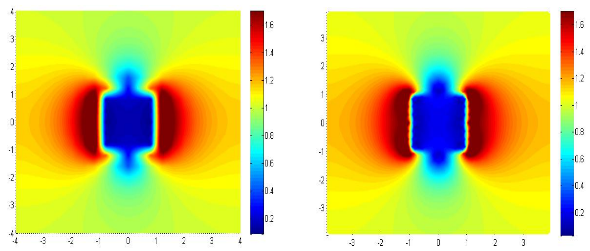


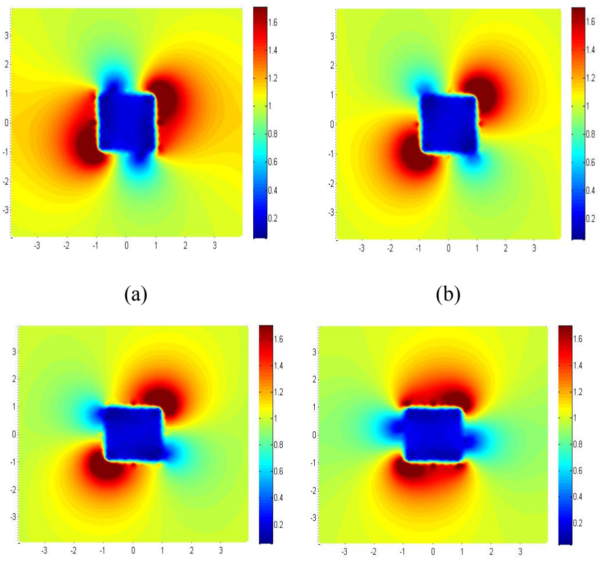
Fig.2 Ag cube model



(a) (b)

Fig.3. Near Field Distribution: (a) FEKO; (b) VIE

Fig. 4(a) ~ (d) shows the electric field distribution of different incident angles. With the change of incident angle, the field enhancement region of nanoarray is also shifted.



(a) (b) (c) (d)

Fig.3. Near Field Distribution for Various Incident Angles: (a) 20° (b) 40° (c) 60° (d) 80°

IV. CONCLUSION

This paper presents an effective analysis method for modeling infinite nanoarray. Instead of the infinite nanoarray, only a nano particle needs to be calculated by the Volume Integral Equation Method with the periodic Green's functions. At last we give the electric field distribution of different incident angles and with the change of incident angle, the field enhancement effect of nanoarray is also shifted. The above example has shown that the method is valid.

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