LAYERED MEDIUM DISCRETE DIPOLE APPROXIMATION

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Abstract

In this work, we improved discrete dipole approximation (DDA) to layered medium by formulating the problem with layered medium Green's functions (LMGFs). In order to calculate thousands of LMGF samples, we subtract the singularities of LMGFs and add their contributions analytically. This new layer medium DDA can solve electromagnetic scattering from arbitrarily shaped objects embedded in a layered medium accurately. Numerical results clearly demonstrate the efficiency of the method with respect to regular DDA and frequency domain full wave solvers.

1 Introduction

Recent developments in nano-fabrication, which allows metals to be structured and characterized on the nanometer scale, make surface plasmons (SPs) attractive to a wide spectrum of engineers and scientists to develop new types of optical antennas, photonic devices and sensors. SPs are simply electromagnetic waves that propagate along the surface of a conductor. Their importance comes from the fact that when periodically located, metal nanoparticles (MNPs) can lead to giant electromagnetic field enhancement. Optical antennas, surface or tip enhanced Raman scattering, and nonlinear frequency generation are some of the current SP applications, in which researchers try to tune up the properties of SPs and their interaction with light according to the problem of interest by changing the shape, size, and material composition of the NPs.

One of the most commonly used fundamental methods to study SP resonance modes of MNPs is the discrete-dipole approximation (DDA) [1, 2]. In DDA, MNPs are approximated as single or sum of oscillating dipoles based on the size of the MNP with respect to the wavelength. This simple method is very efficient in terms of accuracy and CPU time but requires a homogeneous background, which is not typical for a real world SP implementation [3-7]. For example, a typical transmission spectroscopy measurement is carried out with MNPs fabricated on an indium tin-oxide (ITO) coated glass. Here, air/ITO/glass/air establishes a 4-layer structure. Classical DDA solutions differ significantly then the experimental results, because they assume MNPs are situated in a homogeneous medium. Recently Simsek developed an advanced coupled dipole approximation [8] that can handle the inhomogeneous background, but this method is only valid for the particles approximated with a single dipole.

In this work, we developed an advanced DDA method using layered medium Green's functions (LMGFs) [9], namely the layered medium discrete dipole approximation (LM-DDA) to calculate scattering and absorption of light by irregular particles embedded in a multilayered structure. The key ingredient of our approach is use of LMGFs which can be seemed as the impulse response of a multilayered structure. In this approach, LMGFs incorporates the effect of multi-layered background and we apply DDA as if MNPs are situated in vacuum. LM-DDA allows us to investigate the effects of layer interface and different layer combinations.

2 Layered Medium Green's Functions

Consider a general multilayer medium consisting of N layers separated by $N-1$ planar interfaces parallel to the xy plane. Layer i exists between z_i and z_{i-1} and is characterized by permittivity ε_i and permeability μ_i. An arbitrarily directed electric dipole $\mathbf{P}$ can be represented in the cartesian coordinates by $\mathbf{P} = \hat{x}p_x + \hat{y}p_y + \hat{z}p_z$. Similarly, electric field $\mathbf{E}$ created by that dipole can be decomposed as $\mathbf{E} = \hat{x}E_x + \hat{y}E_y + \hat{z}E_z$. The relationship between each component of the field and the dipole is given by the dyadic layered medium Green's functions, $\overline{G}(r,r')$, as follows

$$\begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix} = \begin{bmatrix} G_{xx} & G_{xy} & G_{xz} \\ G_{yx} & G_{yy} & G_{yz} \\ G_{zx} & G_{zy} & G_{zz} \end{bmatrix} \cdot \begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix}. \quad (1)$$

In this notation, $G_{\eta\zeta}$ gives $\hat{\eta}$ component of the electric field at r due to a $\hat{\zeta}$ directed unit electric dipole located at r', where η and ζ are either x, y, or z.

For more detailed information, reader is refered to [8] but here we would like to point out that LMGF's can be written as a sum of primary field term and reflection terms:

$$G_{\eta\zeta} = G_{\eta\zeta}^{prim} + G_{\eta\zeta}^{refl}. \quad (2)$$

3 Layered Medium Discrete Dipole Approximation

Assume an arbitrarily shaped object embedded in a multilayered medium, with *N* layers. The object is

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approximated by *M* dipoles with polarizabilities α_j, located $\mathbf{r}_j$. Each dipole has a polarization $\mathbf{P}_j = \alpha_j\, \mathbf{E}_j$, where $\mathbf{E}_j$ the electric field at $\mathbf{r}_j$ due to incident field $\mathbf{E}_{inc,j}$ plus the contribution of each of the *M-1* dipoles, such that

$$\mathbf{E}_j = \mathbf{E}_{inc,j} - \sum_{\ell\neq j}\overline{G}_{j\ell}\mathbf{P}_\ell. \qquad (3)$$

In fact, Eq. (3) can be written in a more compact form by using $\mathbf{E}_j = \mathbf{P}_j / \alpha_j$. In other words, we can obtain a system of 3N complex linear equations

$$\sum_{\ell=1}^{M}\overline{G}_{j\ell}\mathbf{P}_\ell = \mathbf{E}_{inc,j}. \qquad (4)$$

In free space, polarizability of a MNP along the η-axis (η is x, y, or z) is given by

$$\alpha_\eta^{fs} = \frac{\varepsilon_r - \varepsilon_b}{\varepsilon_r + 2\varepsilon_b} r^3, \qquad (5)$$

where *r* is the radius of the MNP, ε_r and ε_b are the relative permittivity of the MNP and the host medium, respectively. However, the polarizability of the MNP in a layered medium is given by

$$\alpha_\eta^{lm} = \left(\frac{1}{\alpha_\eta^{fs}} - i\frac{2}{3}k^3 - \frac{k^2}{r} - G_{\eta\eta}^{refl}(r_0, r_0)\right)^{-1}, \qquad (6)$$

where *k* is the wavenumber, r_0 is the mass center of the MNP, as explained in [7]. Once we know P_j values, we can calculate near and far fields as explained in [1].

4 Numerical Results

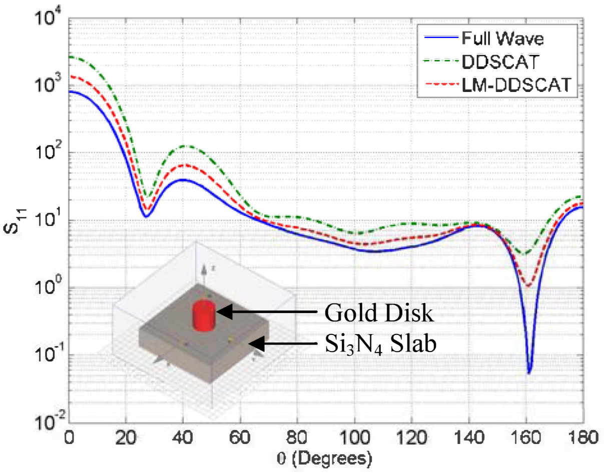

Figure 1 S_{11} values obtained with a full wave solver (blue), DDSCAT (green) and LM-DDSCAT (red) for a gold disk with a radius of λ/8 and a height of λ/2 on top a Si_3N_4 slab with dimensions of 2λ×2λ×λ/2, where λ = 532 nm.

Please see Figure 1 and its caption, which is not detailed here for the sake of brevity. However, we would like to emphasize that LM-DDSCAT solution takes only 43 seconds (and uses 72 MB of RAM) to solve the scattering problem depicted in Figure 1, whereas DDSCAT takes 3900 seconds (and uses 1 GB of RAM) for the same problem.

5 Conclusions

In this work, we implemented discrete dipole approximation with layered medium Green's functions. This new formulation allow us to calculate optical properties of arbitrarily shaped complex objects embedded in layered medium. Numerical results show a very good agreement with the experimental results found in the literature.

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