A Hybrid Spectral Integral - Finite Element Method for Layered Media Including Graphene-like Atomically Thin Layered Materials

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***Abstract*—Layered medium Green's functions (LMGFs) are calculated for a multilayered medium including graphene-like atomically thin layered materials. A spectral integral method (SIM) implemented with LMGFs is used as an exact radiation boundary condition to truncate the computational domain in the finite element method (FEM) to form a hybrid SIM/FEM which is applicable to arbitrary inhomogeneous objects. Numerical studies confirm the accuracy of the method.**

I. Introduction

Graphene has gathered a strong interest both from the research community and industry in the last decade due to its unique electrical and mechanical properties [1]–[9]. It has already found different roles in a wide range of applications including optical modulators [3], transistors [4], p-n junctions [5], sensors [6], waveguides [7], transformation optics [8], LEDs, photodetectors, absorbers, frequency converters, and many other subjects [9]. Similar efforts can be found in the literature for other graphene-like atomically thin layered materials (ATLMs) including nitrides (e.g., hexagonal boron nitride), dichalcogenides (e.g., molybdenum sulfide) and oxides (e.g., vanadium pentoxide).

Although the interest on ATLMs is enormous, there are only a limited number of efforts from the computational electromagnetic community. One of the main reasons behind this lack of response is the use of two-dimensional (2D) optical conductivity (σ_c) to represent ATLMs. Such material modeling requires a special boundary condition wherever the graphene layer is present. Alternatively, 2D optical conductivity can be converted to an effective complex electrical permittivity (ϵ_{eff}) and the ATLM can be treated as a 3D material with ϵ_{eff} and a finite thickness. These two approaches are labeled as 2D and 3D, respectively, in the rest of the paper.

In this work, electromagnetic wave propagation through and scattering from 2D inhomogeneous objects embedded in a multilayered medium, which includes an ATLM, is solved with a hybrid spectral integral method (SIM) - finite element method (FEM). First, layered medium Green's functions (LMGFs) are calculated using modified Fresnel reflection and transmission equations in order to take ATLM into account. Second, SIM implemented with LMGFs is used as an exact radiation boundary condition to truncate the computational domain in the FEM to form a hybrid SIM/FEM which is applicable to arbitrary inhomogeneous objects. Numerical results compare the accuracy two SIM/FEM solvers implemented with σ_c and ϵ_{eff} for the treatment of ATLM.

II. Theory

Consider a general multilayer medium consisting of N layers separated by $N-1$ planar interfaces parallel to the xy plane, as shown in Fig. 1. Layer i exists between z_i and z_{i-1} and is characterized by relative electrical permittivity ϵ_i and relative magnetic permeability μ_i. The top surface of the ith interface is coated with an ATLM.

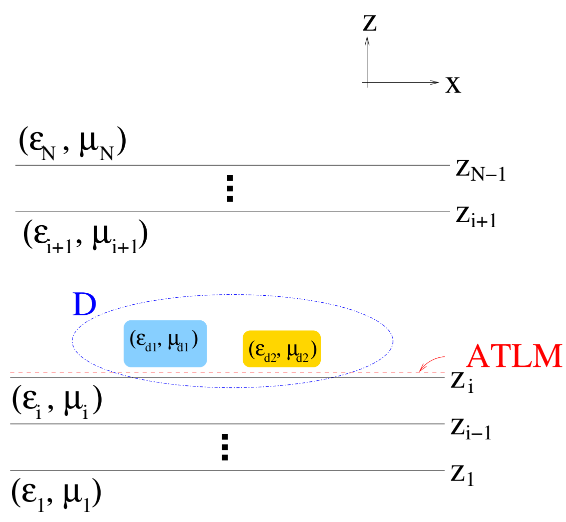

Fig. 1. An N-layer medium with two scatterers and an ATLM on top of the ith interface. Dashed blue line represents an artificial boundary.

Assume there are two homogeneous cylindrical objects embedded in the multilayered medium, represented by ϵ_{dm} and μ_{dm}, where m is either 1 or 2 in Fig. 1, but m can be an arbitrary number.

In order to solve the electromagnetic wave propagation through and scattering from this structure, an artificial boundary, D, is applied to truncate the scatterers from the layered medium. Then, a boundary integral equation on the outside of D is obtained from the 2D Helmholtz equations for the scalar field E_z for the TM_z case (and H_z for the TE_z case) by approximating the unknown field and its derivative by truncated Fourier series [14], [15]. The singular terms in the Green's functions and the non-smooth terms in their derivatives are handled appropriately [15] to maintain high accuracy of SIM.

For the FEM solution of TM_z case, interior region is discretized into triangular elements and linear pyramid basis functions are used to expand the electric field $E_z(x, y)$ in the interior and triangular basis function is used to expand the boundary value $\partial E_z/\partial n$ on D. Additional conditions are provided by the radiation boundary condition. In order to use the SIM as a radiation boundary condition for the FEM, we need to relate the electric field and its normal derivative on the boundary D. The pyramid basis expansion coefficients are obtained by the Fourier coefficients of electric field and its normal derivative on the boundary through trigonometric interpolation [14]. The final set of equations can be solved with a straightforward matrix inversion to obtain electric field and its normal derivative on the boundary D. A similar procedure can be followed for the TE_z case.

In order to take the ATLM into account, one might either follow the 3D approach (by using ϵ_{eff} and a finite thickness) or the 2D approach by using σ_c only to represent the ATLM. For the latter case, the Fresnel reflection coefficients for TM and TE waves from the interface between the layer i and layer $i+1$ should be modified as follows [12]

$$R^{TM}_{i,i+1} = \frac{\epsilon_{i+1}k_{z,i} - \epsilon_i k_{z,i+1} - jk_{z,i}k_{z,i+1}\sigma_c/\omega}{\epsilon_{i+1}k_{z,i} + \epsilon_i k_{z,i+1} - jk_{z,i}k_{z,i+1}\sigma_c/\omega}, \quad (1)$$

$$R^{TE}_{i,i+1} = \frac{\mu_{i+1}k_{z,i} - \mu_i k_{z,i+1} - j\sigma_c\omega}{\mu_{i+1}k_{z,i} + \mu_i k_{z,i+1} + j\sigma_c\omega}. \quad (2)$$

respectively, where $k_{z,i}^2 = k_i^2 - k_\rho^2$, k_i is the wave-number of layer i, k_ρ is the radial wave-number (integration variable of the Sommerfeld integrals).

III. Numerical Results

Assume, there are two gold rectangular cylinders on top of a graphene coated Si/SiO_2 substrate. First cylinder is 90 nm $\times$30 nm and centered at (-55, 15) nm. Second cylinder is 40 nm $\times$30 nm and centered at (30,15) nm. The scatterers are excited with a TM_z plane wave with a wavelength of 633 nm, incident normally to the interface. The relative permittivity of SiO_2 and Si are taken as 2.5 and 12-j0.0005, respectively. SiO_2 layer is 285 nm thick. Conductivity of graphene calculated by using the method provided in [13]. Complex electric permittivity of gold is -9.81-j1.96 based on the experimental results provided [16]. There are 11 receivers linearly spaced along $z = 50$ nm from $x = -100$ nm to $x = 100$ nm. Fig. 2 compares the magnitude of total electric field at the receivers for two different chemical potential values ($\mu_c = 0$ and 0.6 eV). These 2D results agree well with the 3D approach. Details and some discussions on the periodic case will be provided at the conference.

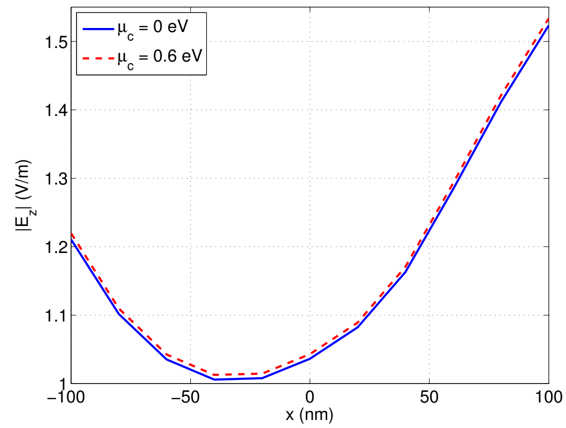

Fig. 2. Blue and red lines show the magnitude of the total electric field (E_z) for $\mu_c = 0$ and $\mu_c = 0.6$ eV, respectively.

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