Three-Dimensional Field-Flux Eigenmode Formulation for Periodic Graphene Structures

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We present a three-dimensional Field-Flux eigenmode Finite Element formulation, able to provide an accurate approximation of the propagation characteristics of periodic structures featuring graphene. The proposed formulation leads to a linear eigenmode problem, where the effective refractive index is the eigenvalue and the electric field intensity and magnetic flux density are the state variables, while graphene's contribution is incorporated via a finite conductivity boundary condition. The formulation is spurious free and can provide accurate dispersion diagrams for an arbitrary propagation direction.

***Index Terms*— Eigenvalues and eigenfunctions, Finite element analysis, Graphene, Periodic structures**

I. Introduction

In the past decade, graphene, the two-dimensional carbon allotrope has attracted significant interest due to its infinitesimally small thickness and its unique characteristics, such as the ability to support highly confined surface plasmon polariton (SPP) propagation at the far infrared regime. In particular, there has been significant interest for applications utilizing the plasmonic properties of graphene with the most prevalent examples being THz waveguides and antennas [1]-[3]. Moreover, structures featuring some kind of periodicity on graphene, either in the form of periodically modulated conductivity or in the form of discontinuities in the graphene surface, have shown great potential in tailoring propagation characteristics and improving the excitation techniques of the graphene plasmonic modes [4]. The purpose of the proposed formulation is to provide a numerical tool for accurate approximation of the propagation characteristics of these periodic structures in terms of the dispersion diagram.

II. Field-Flux Eigenmode Formulation for Periodic Graphene Structures

A. The Field Flux Formulation

The finite element field flux formulation is based on the system of Maxwell's equations solving for both the electric field $\mathbf{E}$ and the magnetic flux $\mathbf{B}$ and follows the framework that has been proposed in [5]. The intrinsic ill-conditioning of this system due to the presence of the μ_0^{-1} and ε_0 coefficients in the Ampere differential equation is improved by scaling the magnetic flux $\mathbf{B}$ using the vacuum wave velocity.

$$\tilde{\mathbf{B}} = -jc_0\mathbf{B}\,. \tag{1}$$

Introducing the scaled magnetic flux into Maxwell's equations results in the scaled system of equations

$$\nabla\times\mathbf{E} = k_0\tilde{\mathbf{B}}\,, \tag{2a}$$

$$\nabla\times\bar{\bar{\mu}}_r^{-1}\tilde{\mathbf{B}} = k_0\bar{\bar{\varepsilon}}_r\mathbf{E}\,, \tag{2b}$$

where k_0 is the vacuum wavenumber and $\bar{\bar{\varepsilon}}_r$, $\bar{\bar{\mu}}_r$ the relative dielectric permittivity and magnetic permeability tensors. The symmetry of structures featuring periodic variances along the propagation axis allows us to reduce the computational space to three-dimensional periodic cell by imposing the Bloch periodic boundary condition on the corresponding port. In addition, by taking into account that graphene's conductivity is a function of the radial frequency and that the lossy nature of graphene renders the propagation length a very important part of the dispersion, we arrive at the conclusion that for the current problem it is much more convenient to calculate the wavenumber as a function of frequency rather than the opposite. Assuming arbitrary propagation direction $\hat{\mathbf{k}}$, the corresponding wave vector can be expressed as $\mathbf{k} = k_0 n_{eff}\hat{\mathbf{k}}$,where n_{eff} the unknown effective refractive index of the wave. Restricting the computational space in the unitary cell of the periodic structure allows us to cast the electric and magnetic fields in Bloch form.

$$\mathbf{E} = \mathbf{e}e^{-jk_0 n_{eff}\hat{\mathbf{k}}\cdot\mathbf{r}}\,, \tag{3a}$$

$$\tilde{\mathbf{B}} = \tilde{\mathbf{b}}e^{-jk_0 n_{eff}\hat{\mathbf{k}}\cdot\mathbf{r}}\,, \tag{3b}$$

where $\mathbf{e}$ and $\tilde{\mathbf{b}}$ the *vectorial* periodic envelopes of the electric and magnetic fields. The periodic envelopes, along with the effective refractive index constitute the state variables of the problem. Restating (2a) and (2b) with respect to the Bloch transformation leads to the modified system of Maxwell's Equations.

$$\nabla\times\mathbf{e} - jk_0 n_{eff}\hat{\mathbf{k}}\times\mathbf{e} = k_0\tilde{\mathbf{b}}\,, \tag{4a}$$

$$\nabla\times\bar{\bar{\mu}}_r^{-1}\tilde{\mathbf{b}} - jk_0 n_{eff}\hat{\mathbf{k}}\times\bar{\bar{\mu}}_r^{-1}\tilde{\mathbf{b}} = k_0\bar{\bar{\varepsilon}}_r\mathbf{e}\,, \tag{4b}$$

This system defines a generalized linear eigenvalue problem in terms of n_{eff}, for which the known operating frequency is inserted via k_0. To apply the Galerkin method on the modified Maxwellian system, equation (4a) is weighed with testing functions for the magnetic flux while equation (4b) is weighed with the testing functions for the electric field:

$$\iiint_\Omega \tilde{\mathbf{b}}'\cdot\nabla\times\mathbf{e}\,dv - k_0\iiint_\Omega \tilde{\mathbf{b}}'\cdot\tilde{\mathbf{b}}\,dv - jn_{eff}k_0\iiint_\Omega \tilde{\mathbf{b}}'\cdot\hat{\mathbf{k}}\times\mathbf{e}\,dv = 0\,, \tag{5a}$$

$$\iiint_{\Omega} \nabla \times \mathbf{e}' \cdot \bar{\bar{\mu}}_r^{-1} \tilde{\mathbf{b}} dv + \oiint_{d\Omega} \mathbf{e}' \cdot \hat{\mathbf{n}}_{ext} \times \bar{\bar{\mu}}_r^{-1} \tilde{\mathbf{b}} ds - k_0 \iiint_{\Omega} \mathbf{e}' \bar{\bar{\varepsilon}}_r \mathbf{e} dv$$
$$- jn_{eff} k_0 \iiint_{\Omega} \mathbf{e}' \cdot \hat{\mathbf{k}} \times \bar{\bar{\mu}}_r^{-1} \tilde{\mathbf{b}} dv = 0 , \quad (5b)$$

where $\hat{\mathbf{n}}_{ext}$ is the normal unit vector pointing outward from the boundary surface.

B. Implementation of graphene

Owing to its extremely small thickness, graphene can be regarded as an ideal two-dimensional surface. This allows interpreting its contribution to the overall electromagnetic system as surface current density, which in turn can be treated computationally as a finite conductivity boundary condition, which can be written in the form

$$\hat{\mathbf{n}}_g \times \bar{\bar{\mu}}_r^{-1} \tilde{\mathbf{b}}^{+} - \hat{\mathbf{n}}_g \times \bar{\bar{\mu}}_r^{-1} \tilde{\mathbf{b}}^{-} = -j\eta_0 \sigma_g \mathbf{e}_{tg} , \quad (6)$$

where $\hat{\mathbf{n}}_g$ is the unit vector normal to the graphene surface, σ_g is graphene's conductivity and η_0 the intrinsic impedance of free space. The subscript "t" denotes field components that are tangent on graphene's surface. This interface condition is inserted in the overall problem by substituting (6) in the surface integral term of (5b):

$$\iint_{S_g} \mathbf{e}' \cdot (\hat{n}_{ext} \times \hat{\mu}_r^{-1} \tilde{\mathbf{b}}) ds = j\eta_0 \iint_{S_g} \mathbf{e}'_{tg} \cdot \sigma_g \mathbf{e}_{tg} ds . \quad (7)$$

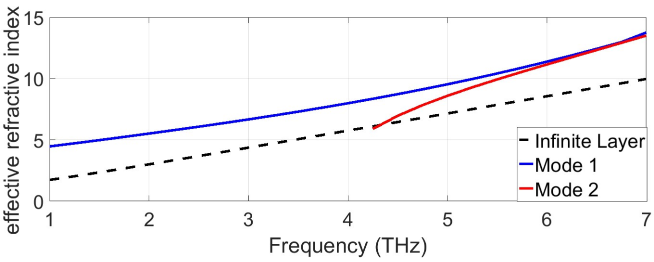

Fig. 1. Dispersion curves of the first two modes of a 5um graphene microribbon compared to the infinite layer.

III. Computational Results

To validate the proposed formulation we examine the well-documented case of a free standing graphene ribbon of 5um width. Graphene's conductivity was evaluated via the Kubo formula at room's temperature $T = 300\text{K}$ with the energy independent scattering rate Γ equal to 0.1meV, the chemical potential equal to 0.2eV. The dispersion diagram of the first two modes supported by the graphene ribbon, compared with the theoretical dispersion of the infinite layer [2] is shown in Fig. 1. Examination of the dispersion of these modes reveals the highly confined nature of the graphene SPPs, as the higher effective index is related with the confinement of moving charges. The distribution of normal and tangential E-field components at the transverse plane on the propagation axis for the first and the second mode are depicted in Fig. 2 and Fig. 3 respectively. In both cases, the concentration of the electric field on the graphene surface is evident. Finally, the dispersion diagram as well as the distribution of the electric field are in accordance with the existing literature [1], [6] and thus validate the accuracy of the proposed formulation.

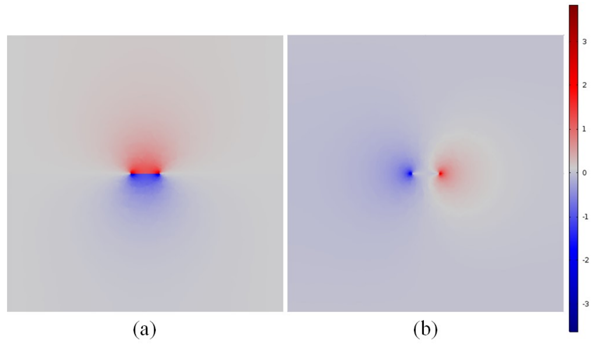

Fig. 2. Distribution of the normal (a) and tangential (b) electric field at the transverse plane on the propagation axis of the first mode at 1 THz.

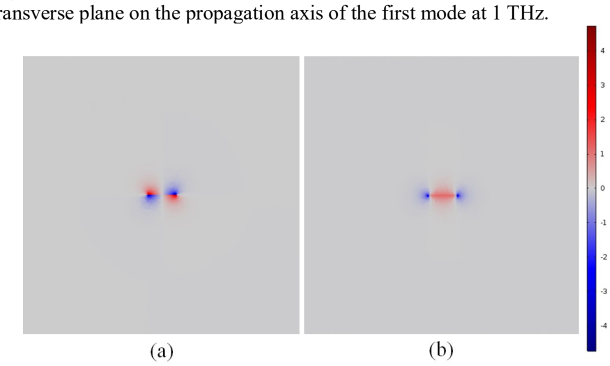

Fig. 3. Distribution of the normal (a) and the tangential (b) electric field at the transverse plane on the propagation axis of the second mode at 4.5 THz.

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