Finite-Difference Frequency-Domain Method Simulates EM Wave Propagation Properties of Parallel Plate Waveguide with Graphene and SiO_2 Layers

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Abstract: *Graphene draws massive interests due to its outstanding physical properties. In recent years, extensive studies have shown its promising features in terahertz (THz) and infrared frequency ranges. However, the EM properties of graphene in the microwave and millimeter wave range are still not well understood. In this paper, we employed finite difference frequency domain (FDFD) method with non-uniform grid to simulate the electromagnetic (EM) behavior of parallel plate waveguides (PPWG) with graphene and a silicon dioxide (SiO_2) buffer layer at 300 GHz. It is shown that the EM wave can be modulated with the presence of the graphene layer. In order to verify the accuracy of the numerical method, the simulated results are compared with analytical calculations. The agreement of numerical and theoretical studies proves that EM wave propagation properties of PPWG can be modulated by changing buffer thickness or by electrically biasing the grapheme layer. This feature of graphene can be used to design new type of EM devices, such as, compact electrically tunable phase shifters or amplitude modulators.*

I. Introduction

Graphene's conductivity can be tuned by either electrostatic or magneto-static gating. The reconfiguration capabilities of graphene electronic properties by applying an external voltage have triggered various studies of graphene based electronic devices [1-4]. Most investigations on graphene devices have been done at infrared and terahertz frequencies and illustrated the advantages of graphene. EM properties of graphene based devices at microwave and millimetre waves are still not well known, even though some recent studies at these frequencies have been reported [5-7].

PPWG supports quasi-transverse electromagnetic (quasi-TEM) modes, and dispersive Transverse electric (TE) and transverse magnetic (TM) modes, and is easy to theoretically analyze because of the regular and simple structure. It is usually chosen to study EM propagation properties of graphene based structures [8-9]. Here we use FDFD method [10] to investigate dispersive TE mode propagation properties of PPWG with graphene and SiO_2 layers at sub-Terahertz frequency. The thickness of graphene is very small compared to the size of PPWG at this frequency, which forms multi-scale problem. In order to solve the problem, non-uniform grid technique is introduced to model the structure.

II. Formulation of FDFD Modelling PPWG with Graphene Layer

A. EM properties of graphene

The conductivity of graphene consists of two parts, intraband and interband [11]. For the case considered here, the intra-band term dominates and can be evaluated as

$$\sigma = \sigma_{\text{int}ra} = -j\frac{e^2 k_B T}{\pi\hbar^2(\omega - j\tau^{-1})}\left(\frac{\mu_c}{k_B T} + 2\ln(e^{-\frac{\mu_c}{k_B T}} + 1)\right) \tag{2}$$

where k_B is Boltzmann's constant, T is temperature, ω is radian frequency, μ_c is chemical potential, τ is a phenomenological electron relaxation time, $-e$ is the charge of an electron, $\hbar$ is the reduced Planck's constant.

B. PPWG with graphene and SiO_2 layers

PPWG incorporating SiO_2 layer and graphene layer is shown as Fig. 1. The graphene layer and SiO_2 layer with thickness d are placed sequentially. The gap with thickness d_{air} between graphene layer and lower metallic plate is filled with air. The structure along the x direction is isotropic and reaches infinite. So the three-dimensional structure can be simplified into a two-dimensional one by reducing the x-axis. The wave propagation direction is chosen as z-axis direction. The dispersive TE modes are considered here.

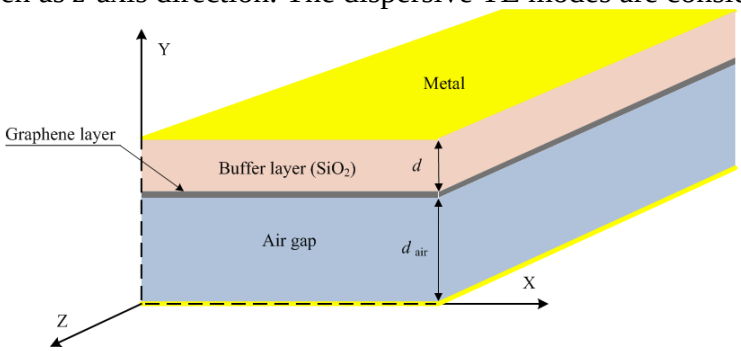


Fig. 1. Schematic diagram of PPWG with graphene and SiO2 layers

The electric field wave equation for 2-D TE_z case in PPWG is

$$\frac{\partial^2 E_x}{\partial y^2} + \frac{\partial^2 E_x}{\partial z^2} = -\omega^2 \varepsilon_e \mu E_x \tag{3}$$

where ω is angular frequency, ε_e and μ are equivalent permittivity and permeability, respectively. ε_e is devoted by permittivity ε and conductivity σ. Along z direction, the electric field component E_x has the form $E_x = E(y)e^{-jk_z z}$. k_z is z-direction wave vector component. Substituting E_x into (3) and eliminating the second partial derivative term, we simplify further the electric field wave equation into one dimension

$$\left(\frac{\partial^2}{\partial y^2} + k^2\right)E_x = k_z^2 E_x \tag{4}$$

where k is wavenumber, $k = \omega^2 \varepsilon\mu$.

C. FDFD method

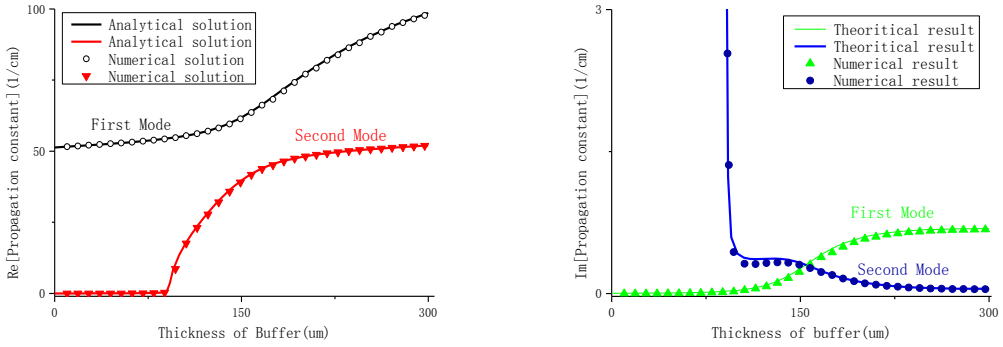
In order to solve equation (4), we employ the FDFD method to discretize the second order partial derivative and derive numerical solutions. As the graphene layer with 0.34 nm thickness is very thin, one-dimensional non-uniform grids [12] are used to model the PPWG structure. The numerical solution of equation (4) in matrix form is

$$[A]\{E_x\} = k_z^2\{E_x\} \tag{6}$$

Obviously, k_z^2 is the Eigenvalue of matrix *A*. Hence we can obtain the propagation wave vectors and their corresponding electric fields by solving the Eigenvalues of matrix *A*.

III. Results of Numerical Simulation and Discussion

Using the FDFD method simulates the EM wave propagation properties of TE_z modes for the detail structure shown in Fig. 1. The thickness of air gap is 0.864 mm, and of graphene layer 0.34 nm, the operating frequency is 300 GHz, the relative permittivity of SiO_2 is 4+0.04*j*. Minimum two TE_z modes, whose dispersion is dependent on the buffer layer thickness, are calculated.



(a) (b)

Fig.2. The lowest two TE modes complex propagation constants of PPWG versus SiO_2 layer thickness *d* in the absence of graphene layer; (a) Real part of complex propagation constant; (b) Imaginary part of complex propagation constant.

Fig.2 (a) and (b) depict the real and imaginary parts of the complex propagation constants, respectively. The good agreement between numerical results and analytical results [13, 14] validates the accuracy of numerical method FDFD. As the thickness of buffer layer increases larger than 90 um, the second mode is excited, and energy coupling between TE_{01} and TE_{02} modes happens.

For the case of PPWG with graphene and SiO_2 layer, τ = 0.5 ps, μ_c = 0.14 eV, and T = 300 K. The minimum size of non-uniform grids is half of graphene thickness.

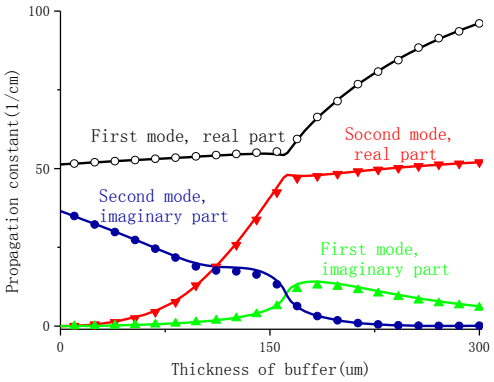


Fig.3. Dependences of the lowest two TE waveguide modes wave vector real and imaginary parts versus SiO2 layer thickness d for graphene electrons Fermi energy equal to 0.14 eV.

Black and green lines are for the real and imaginary parts of the first TE_z mode propagation constant, respectively; red and blue lines shown in Fig.3 are for the real and

imaginary parts of the second TE_z mode propagation constant, respectively. Solid lines are analytical results, and marks are simulated results. The simulated results also agree well with analytical results. For the second TE_z mode, real part of the propagation constant is increasing with increasing of buffer thickness; at the same time, imaginary part of the propagation constant is decreasing with increasing of buffer thickness, which means that the second TE_z mode is excited and modulated by changing thickness of buffer layer when graphene is sandwiched between air gap and buffer layer.

Conclusion

The FDFD method simulating the EM wave propagation properties of a PPWG with graphene layer is validated by comparison with analytical solutions. By introducing graphene into PPWG, higher TE modes, such as TE_{02} mode is excited. Dispersive TE modes can be modulated by tuning the buffer thickness or electrically biasing the grapheme layer. What we have to point out is that, in order to investigate energy coupling happened in the modulation of EM wave propagation, more modes should be taken into consideration.

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