A Hybrid Implicit-explicit FDTD Method to simulate the MDGDM Nanostructure

Yuan-Guo Zhou, *Member, IEEE*, Li Li, Aote Zhang, Tianling Wang, and Xiaobing Han, *Member, IEEE*
Department of Communication and Information Engineering,
Xi'an University of Science and Technology, Xi'an, China
zyg@xust.edu.cn

***Abstract*-A hybrid implicit-explicit finite-difference time- domain method is employed to simulate a graphene-based nanostructure. As the time-step size of the proposed method is only determined by two space discretization, this method is more efficient than conventional FDTD method for simulating structure with thin unit cell. Numerical experiments validate the proposed method, and a novel graphene optical absorber is investigated in this work.**

***Keywords*-hybrid implicit-explicit FDTD, time step, graphene absorber, nanostructure.**

I. INTRODUCTION

The Finite-difference time-domain (FDTD) method has been proved and viewed as a useful tool to give accurate predictions of behaviors for electromagnetic problems [1]. However, because the Courant–Friedrich–Levy (CFL) condition which limits the time-step size in explicit FDTD method has to be satisfied in the first place, the conventional FDTD method has the serious problem of restriction in terms of the time-step size [2]. To overcome this issue, a hybrid implicit-explicit finite-difference time-domain (HIE-FDTD) method has been proposed and developed. The HIE-FDTD is weakly conditionally stable [3], which is extremely useful for the problems with a very fine mesh in one direction. As a result, this method has great advantage for simulation of structure with thin unit cell, such as nanostructure with graphene absorber [4].

On the other hand, graphene has recently brought lots of attention to scientific communities due to its unique properties. In the field of terahertz spectra, for instance, graphene has been widely employed for developing advanced nanophotonic and nanoelectronic devices [5]. In terahertz and infrared regions, graphene can generate surface plasmon polarities (SPPs) and lead to strong light-graphene interactions. However, in the visible and near-infrared range, because of wavelength independent absorption, suspended graphene does not show spectral selectivity. In order to improve the light-interaction, graphene has been proposed to combine with plasmonic nanostructures based on noble metals for improving performance of these nanophotonic devices [6], [7].

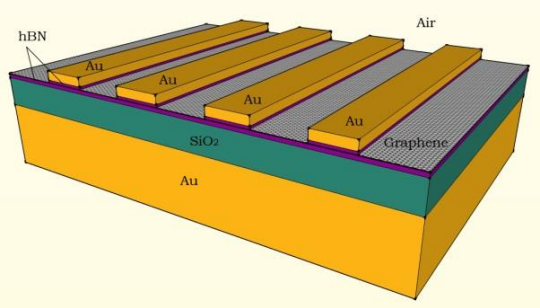

Fig. 1. Schematic drawing of an MDGDM nanostructure

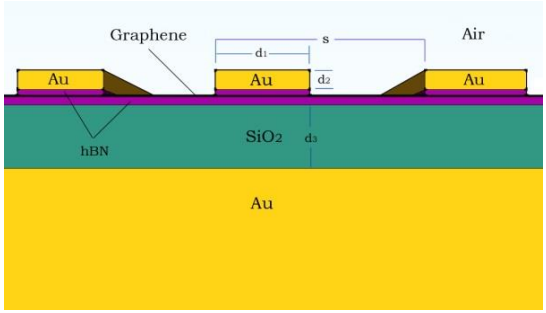

Fig. 2. A front view of the MDGDM nanostructure

In this work, an efficient HIE-FDTD method is proposed to design graphene-based meal-dielectric-graphen-dielectric -metal (MDGDM) nanostructure, which takes advantage of a metal-dielectric-metal (MDM) perfect light absorber. The MDGDM nanostructure comprises periodic gold nanoribbons on a SiO_2 layer coated with graphene supported by a flat gold substrate, and the graphene is sandwiched between two hexagonal boron nitride (h-BN) layers with 2nm thickness, as illustrated in Fig.1 and Fig. 2. The adjustable parameters d_1 and d_2 are the width and thickness of the gold nanoribbon, respectively, which act as insulating spacers to keep higher carrier mobility of grephene and prevent carrier

transport between metal nanoribbons and graphene. The adjustable parameter d_3 is the thickness of SiO_2. The distance between adjacent gold nanoribbons is indicated as parameter $s = 120$ nm. The separation between adjacent nanoribbons is fixed to be relativity large than their width in order to ignore the electromagnetic coupling between nanoribbons. Through HIE-FDTD method, the MDGDM nanostructure is investigated in the remainder of the paper.

II. Update Equations

In the MDGDM scheme, the graphene is described as a significantly thin conducting material with its thickness of 0.34 nm in the *z*-direction. Therefore, with a very fine mesh in this direction, the hybrid implicit-explicit difference scheme is applied, and the iterative formulations of the HIE-FDTD method can be expressed as follows

$$\frac{\varepsilon}{\Delta t}\left[E_y\Big|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}} - E_y\Big|_{i,j+\frac{1}{2},k}^{n-\frac{1}{2}}\right] = \frac{1}{\Delta z}\left[H_x\Big|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n} - H_x\Big|_{i,j+\frac{1}{2},k-\frac{1}{2}}^{n}\right] - \frac{1}{\Delta x}\left[H_z\Big|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n} - H_z\Big|_{i-\frac{1}{2},j+\frac{1}{2},k}^{n}\right] \quad (1)$$

$$\frac{\mu}{\Delta t}\left[H_y\Big|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} - H_y\Big|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n-\frac{1}{2}}\right] = -\frac{1}{\Delta z}\left[E_x\Big|_{i+\frac{1}{2},j,k+1}^{n} - E_x\Big|_{i+\frac{1}{2},j,k}^{n}\right] + \frac{1}{\Delta x}\left[E_z\Big|_{i+1,j,k+\frac{1}{2}}^{n} - E_z\Big|_{i,j,k+\frac{1}{2}}^{n}\right] \quad (2)$$

$$\frac{\varepsilon}{\Delta t}\left[E_x\Big|_{i+\frac{1}{2},j,k}^{n+1} - E_x\Big|_{i+\frac{1}{2},j,k}^{n}\right] = -\frac{1}{\Delta z}\left[H_y\Big|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} - H_y\Big|_{i+\frac{1}{2},j,k-\frac{1}{2}}^{n+\frac{1}{2}}\right] - \frac{1}{2\Delta y}\left[H_z\Big|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+1} - H_z\Big|_{i+\frac{1}{2},j-\frac{1}{2},k}^{n+1} + H_z\Big|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n} - H_z\Big|_{i+\frac{1}{2},j-\frac{1}{2},k}^{n}\right] \quad (3)$$

$$\frac{\varepsilon}{\Delta t}\left[E_z\Big|_{i,j,k+\frac{1}{2}}^{n+1} - E_z\Big|_{i,j,k+\frac{1}{2}}^{n}\right] = \frac{1}{\Delta x}\left[H_y\Big|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} - H_y\Big|_{i-\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}}\right] - \frac{1}{2\Delta y}\left[H_x\Big|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+1} - H_x\Big|_{i,j-\frac{1}{2},k+\frac{1}{2}}^{n+1} + H_x\Big|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n} - H_x\Big|_{i,j-\frac{1}{2},k+\frac{1}{2}}^{n}\right] \quad (4)$$

$$\frac{\mu}{\Delta t}\left[H_z\Big|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+1} - H_z\Big|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n}\right] = -\frac{1}{\Delta x}\left[E_y\Big|_{i+1,j+\frac{1}{2},k}^{n+\frac{1}{2}} - E_y\Big|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}}\right] + \frac{1}{2\Delta y}\left[E_x\Big|_{i+\frac{1}{2},j+1,k}^{n+1} - E_x\Big|_{i+\frac{1}{2},j,k}^{n+1} + E_x\Big|_{i+\frac{1}{2},j+1,k}^{n} - E_x\Big|_{i+\frac{1}{2},j,k}^{n}\right] \quad (5)$$

$$\frac{\mu}{\Delta t}\left[H_x\Big|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+1} - H_x\Big|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n}\right] = \frac{1}{\Delta z}\left[E_y\Big|_{i,j+\frac{1}{2},k+1}^{n+\frac{1}{2}} - E_y\Big|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}}\right] - \frac{1}{2\Delta y}\left[E_z\Big|_{i,j+1,k+\frac{1}{2}}^{n+1} - E_z\Big|_{i,j,k+\frac{1}{2}}^{n+1} + E_z\Big|_{i,j+1,k+\frac{1}{2}}^{n} - E_z\Big|_{i,j,k+\frac{1}{2}}^{n}\right] \quad (6)$$

where *E* and *H* denote the electric field and the magnetic field, respectively. Δx, Δy and Δz are the spatial cell sizes in the *x*-, *y*- and *z*-directions, respectively. Subscript *i*, *j*, *k* denote the corresponding indices of the spatial increment. *n* and Δt are the index and size of the time step, respectively.

Since the HIE-FDTD method is adopted in this work, the CFL condition reduced to weakly conditionally stability and the time step is only determined by these two space discretizations. The limitation for time–step size can be calculated as

$$\Delta t \le 1/c\sqrt{\left(1/\Delta x\right)^2 + \left(1/\Delta y\right)^2} \quad (7)$$

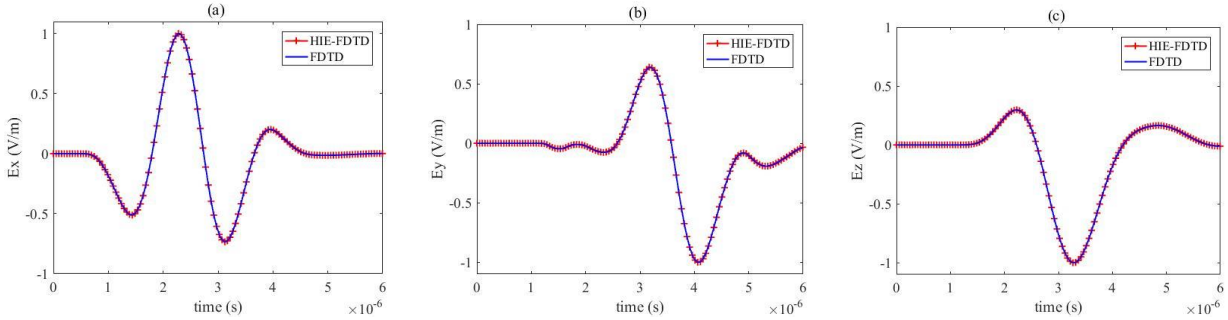

Fig. 3. (*a*)-(*c*) the comparison of electric field three components obtained by HIE- FDTD and conventional FDTD method

III. Numerical Simulation

To test the computational accuracy of the proposed method, a comparison is made between HIE-FDTD and conventional FDTD. Electric fields at the observation point *F* that is 15 nm away from the graphene sheet are shown in Fig. 3. We notice that the proposed method demonstrates very good agreement with the conventional method without introducing additional cost of simulation time and storage memory. The detail comparison of electric field components

E_x, E_y and E_z are illustrated in Fig. 3(*a*), 3(*b*) and 3(*c*), respectively.

Under illumination of normal incident light, we investigate the optical absorption of graphene in the MDGDM nanostructure, and the absorption spectrum is illustrated in Fig. 4.

The reflection coefficient R is defined as

$$R = \left| E_r / E_{in} \right| \quad (8)$$

Here, E_r is the reflection electric field at the observation point and E_{in} is the incident electric field. The absorption rate A is expressed as

$$A = 1 - \left| R \right|^2$$

The nanoribbon acts as a resonator for the horizontal plasmon guided mode, therefore, the resonant wavelength is very sensitive to the nanoribbon width d_1. As demonstrated in Fig. 4(*a*), when d_1 increases from 30 nm to 50 nm, the absorption rate of graphene drops due to the increment of the effective resonance wavelength of the localized surface plasmon.

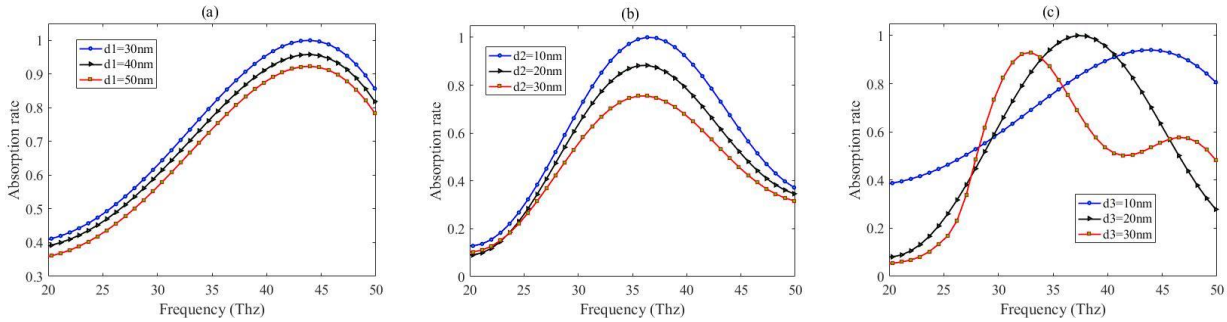

Fig. 4. (*a*)–(*c*) absorption spectra of graphene under illumination of normal incident light.

Next, we discuss effects of changing the nanoribbon thickness d_2 on the absorption of graphene. As shown in Fig. 4(*b*). When d_2 increases from 10 nm to 30 nm, the absorption rate of graphene also drops because of enhancement of the wave diffraction around the gold nanoribbons. In addition, since the resonance properties of MDGDM nanostructures are highly sensitive to the thickness variation of the dielectric spacer layers, the tuning of absorption band of graphene will be greatly facilitated by slightly changing the spacer thickness d_3, as illustrated in Fig. 4(*c*).

IV. Conclusions

In this paper, a HIE-FDTD method for analyzing graphene absorption in the MDGDM nanostructure is proposed. Meanwhile, by the proposed method we have investigated the optical properties of the structures for light energy harvesting in graphene. A series of numerical experiments are carried out and the results show the potential application in novel graphene-based optoelectronic devices.

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