Effective Modeling of Tunable Graphene with Dispersive FDTD - GSTC Method

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Abstract — We propose an effective method of dispersive finite difference time domain-generalized sheet transition conditions (FDTD-GSTCs) for the modeling of electromagnetic fields from tunable graphene with nearly zero thickness. To model the tunable graphene effectively, the susceptibilities are introduced instead of its physical structure, which can be extracted from reflection or transmission coefficients. In order to model the graphene in broadband, a dispersive FDTD-GSTC method is introduced by fitting the susceptibilities with respect to frequencies with the complex-conjugate pole-residue (CCPR) pairs. Numerical results demonstrate the validity of the proposed method.

Index Terms — Broadband, dispersive, finite difference time domain, graphene.

I INTRODUCTION

Graphene has a wide range of applications due to its excellent conductivity, good thermal stability, high electron mobility, low density, promising wave absorbing material, and easy to be tunable with biasing electrostatic or a magnetostatic field [4]. To simulate it with typical three-dimensional numerical methods will lead to very low computation efficiency [5]-[10], due to its single atom thickness. To model the thin graphene layer effectively, many techniques such as the thin dielectric sheet (TDS) [5], surface impedance boundary condition [6], sub-cell discretization technique [7], and hybrid time domain implicit–explicit method [8] are widely developed.

In recent years, generalized sheet transition conditions (GSTCs) have been widely used in the analysis of electromagnetic metasurfaces [11]-[13]. In this work, we extend the GSTC for the modeling of metasurface [17] with graphene. The complex-conjugate pole-residue (CCPR) pairs method [3] is proposed to fit the dispersive susceptibility tensors for the analysis of the wideband electromagnetic property of graphene sheet.

This paper is organized as follows: Section II briefly describes the FDTD-GSTC method; Section III describes the dispersive FDTD-GSTC method in detail; numerical simulations of tunable graphene in Section IV validate the proposed method. Finally, a short conclusion is given in Section V. The results of this work are initially presented at the 2018 ACES-China conference in Beijing [16].

II FDTD-GSTC METHOD

As shown in Fig. 1, the graphene is located at $xoy$ plane, the boundary conditions can be written as [1], [11]:

$$\begin{align*}
\hat{z} \times \Delta H &= j \omega P - \hat{z} \times \nabla M_z, \\
\Delta E \hat{z} &= j \omega \mu M - \nabla \left( \frac{P_z}{\varepsilon} \right) \times \hat{z}, \\
\hat{z} \cdot \Delta D &= -\nabla \cdot P, \\
\hat{z} \cdot \Delta B &= -\mu \nabla \cdot M,
\end{align*}
$$

where $P$ and $M$ are the electric and magnetic surface polarization densities, respectively. $\Delta H$ and $\Delta E$ represent the difference of electromagnetic field on the two sides of the graphene.

![Graphene located at $xoy$ plane.](image)

The electric and magnetic polarization current densities are defined as [1], [11]:

$$\begin{align*}
P &= \varepsilon \chi_{ee} \mathcal{E}_{aw} + \frac{\varepsilon}{\chi_{em}} \sqrt{\mu} H_{aw}, \\
M &= \frac{\varepsilon}{\chi_{em}} H_{aw} + \frac{\varepsilon}{\chi_{ew}} \sqrt{\mu} E_{aw},
\end{align*}
$$

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where $\overline{\chi}_{ee}$, $\overline{\chi}_{en}$, and $\overline{\chi}_{em}$ are susceptibility tensors. $E_{av}$ and $H_{av}$ are the average value of electromagnetic field on the two side of the graphene.

In the particular case, we assume that the normal electric and magnetic polarization currents of graphene are zero, i.e., $P_i = 0$ and $M_j = 0$. So that the susceptibility tensors reduce to $2 \times 2$ transverse tensors. Substituting Eq. (2) into Eq. (1), we can obtain [2]:

$$
\begin{align}
\left( -\Delta \hat{H}_y \right) &= j\omega \mu \left( \chi_{ee} \hat{E}_{av} + \chi_{en} \hat{E}_{av} \right), \\
\left( \Delta \hat{H}_y \right) &= j\omega \mu \left( \chi_{en} \hat{E}_{av} + \chi_{ee} \hat{E}_{av} \right),
\end{align}
$$

with Eq. (3a) without loss of generality, we assume the elements are monoanisotropic and non-gyrotropic ($\chi_{ee}$, $\chi_{en}$, $\chi_{em}$, $\chi_{en}$, $\chi_{en}$, and $\chi_{em}$ are equal to zero). Since the sheet is infinitesimal thin, there are no normal components of the charges and currents. As a result, the time domain expression of Eq. (3) can be simplified as:

$$
\begin{align}
J_y &= \Delta H_y = e_0 \chi_{ee} \frac{\partial E_{av}}{\partial t}, \\
J_x &= \Delta H_y = e_0 \chi_{en} \frac{\partial E_{av}}{\partial t}, \\
K_x &= \Delta E_x = \mu_0 \chi_{en} \frac{\partial H_{av}}{\partial t}, \\
K_y &= \Delta E_x = \mu_0 \chi_{ee} \frac{\partial H_{av}}{\partial t},
\end{align}
$$

where $J_p = j\omega P_p$ and $K_p = j\omega \mu_0 M_p$ with $p = x, y$ represent the polarization electric and magnetic current densities, respectively. When we insert it into the Ampere’s and Faraday’s laws, the FDTD updating equations as in Eq. (5) can be obtained. It can be found from Eq. (4), when the polarization susceptibilities are related to the frequencies, careful treatment of a dispersive FDTD-GSTC should be derived as will be presented in Section III.

### III. DISPERSIVE FDTD-GSTC METHOD WITH CCPR PAIRS

The susceptibility tensors can be extracted from the reflection and transmission coefficients [1], as a result, the susceptibility tensors are related to frequencies. In this work, the broadband susceptibilities with respect to frequencies can be fitted with the complex-conjugate pole-residue (CCPR) pairs [3]. Hence, the susceptibility tensors can be approximated as:

$$
\chi(\omega) = d + \sum_{p=1}^{N} \left( \frac{c_p}{j\omega - a_p} + \frac{c_p^*}{j\omega - a_p^*} \right),
$$

where $d$ is a constant term, $(a_p, c_p)$ and $(a_p^*, c_p^*)$ are the complex-conjugate pole-residue pairs, respectively. With CCPR pairs, the polarization electric and magnetic current densities can be separated into the constant term and dispersive term:

$$
\begin{align}
J &= J_{dis} + J_{con}, \\
K &= K_{dis} + K_{con},
\end{align}
$$

where $J_{con}$ and $K_{con}$ represent constant term of electromagnetic current density. $J_{dis}$, $J_{con}$, $K_{dis}$, and $K_{con}$ represent two complex-conjugate pair current terms [3].

Fig. 2. A flowchart of FDTD-GSTC.

The constant term of equivalent surface currents on the graphene sheet can be solved by the traditional FDTD method [14], [15]. While the dispersive term of equivalent surface currents can be expressed by CCPR [3]:

$$
\begin{align}
J_{p_{-dis}} &= e_0 \frac{c_p}{j\omega - a_p} j\omega E, \\
K_{p_{-dis}} &= \mu_0 \frac{c_p}{j\omega - a_p} j\omega H.
\end{align}
$$

Assuming the graphene is located at cell of $(i, j, p)$, Eq.
(8) in can be written in a discrete form:

\[
\mathbf{J}^{n}_{p,\text{dis}} = k_p \mathbf{J}^{n-1}_{p,\text{dis}} + b_p \frac{E^n - E^{n-1}}{\Delta t}, \quad (9a)
\]

\[
\mathbf{K}^{n}_{p,\text{dis}} = k_{kp} \mathbf{K}^{n-1}_{p,\text{dis}} + b_{kp} \frac{H^n - H^{n-1}}{\Delta t}, \quad (9b)
\]

where \( k_p = \frac{2 + a_p \Delta t}{2 - a_p \Delta t} \), \( b_p = \frac{a_0 c_p 2 \Delta t}{2 - a_p \Delta t} \), \( k_{kp} = \frac{2 + a_{kp} \Delta t}{2 - a_{kp} \Delta t} \), and \( b_{kp} = \frac{\mu_0 c_{kp} 2 \Delta t}{2 - a_{kp} \Delta t} \).

After this, we can substitute the current densities of (9) into (5), finally, the updating equation of \( E_y \) and \( H_z \) at cell \((i, j, p)\) based on the Yee grid can be obtained as in Eqs. 10 (a) and (b). Similarly, \( E_x \) and \( H_y \) can be obtained as in Eqs. 10 (c) and (d). It should be noted here, for single layer graphene sheet without substrate \( \Delta E = 0 \), thus there is no need to update the magnetic equations in FDTD. The flowchart of the proposed FDTD-GSTC is shown in Fig. 2.

\[
E_x(i, j, p) = E_x^{n-1}(i, j, p) + \frac{\Delta t}{\varepsilon_0} \left[ \frac{\varepsilon_0 \Delta z}{\Delta z} \sum_{p=1}^{N} \text{Re}(b_p) + d_{0} \varepsilon_0 \right] \left[ E_x^n(i, j, p) - E_x^{n-1}(i, j, p) - H_y^n(i, j, p) - H_y^{n-1}(i, j, p) \right]
\]

\[
H_y(i, j, p) = H_y^{n-1}(i, j, p) + \frac{\Delta t}{\mu_0} \left[ \frac{\mu_0 \Delta z}{\Delta z} \sum_{p=1}^{N} \text{Re}(b_p) + d_{1} \mu_0 \right] \left[ E_x^n(i, j, p) - E_x^{n-1}(i, j, p) - H_y^n(i, j, p) - H_y^{n-1}(i, j, p) \right]
\]

\[
E_y(i, j, p) = E_y^{n-1}(i, j, p) + \frac{\Delta t}{\varepsilon_0} \left[ \frac{\varepsilon_0 \Delta z}{\Delta z} \sum_{p=1}^{N} \text{Re}(b_p) + d_{0} \varepsilon_0 \right] \left[ H_x^n(i, j, p) - H_x^{n-1}(i, j, p) - E_y^n(i, j, p) - E_y^{n-1}(i, j, p) \right]
\]

\[
H_x(i, j, p) = H_x^{n-1}(i, j, p) + \frac{\Delta t}{\mu_0} \left[ \frac{\mu_0 \Delta z}{\Delta z} \sum_{p=1}^{N} \text{Re}(b_p) + d_{1} \mu_0 \right] \left[ H_x^n(i, j, p) - H_x^{n-1}(i, j, p) - E_y^n(i, j, p) - E_y^{n-1}(i, j, p) \right]
\]

IV NUMERICAL RESULTS

In this section, numerical simulations of graphene are shown to demonstrate the validity of the proposed dispersive FDTD-GSTC method, all the simulations are carried out on a personal computer of Intel(R) Core(TM) i3-4170 CPU with 3.7GHz and 16 GB RAM. We use Fortran to code the proposed algorithm.

A graphene with cross-shaped elements

Firstly, the graphene with cross-shaped elements is simulated, as inset in Fig. 3 (b), the dimensions of the element are: \( L = 48\mu m, d_1 = d_2 = 6\mu m \), and the period of...
the array is 60 \text{um}. The scattering rate of graphene sheet is 0.5 meV, the temperature is 300 K, and the biasing electric field is of 2V/nm. With the complex-conjugate pole-residue pairs method, the broadband (0.1 THz to 2 THz) susceptibilities with respect to frequencies can be fitted well as shown in Fig. 3 (a). Here, four terms are employed, and the coefficients of them are listed in Table 1, respectively.

![Graphene sheet simulation](image)

**Fig. 3. Simulation of cross-shaped graphene with periodic boundary condition:** (a) broadband susceptibility $\chi^{xx}_{ee}$ fitted by complex-conjugate pole-residue pairs, and (b) reflection coefficient by commercial software and proposed FDTD-GSTC method.

With the proposed dispersive FDTD-GSTC, the mesh size can be $dx = dy = dz = 2\text{um}$, which is much larger than conventional FDTD method [14], [15]. Figure 3 (b) plots the simulated reflection coefficients of the proposed dispersive FDTD-GSTC method and commercial software HFSS, very good agreement can be found. The simulation time and memory of FDTD and FDTD-GSTC are listed in Table 2. It can be seen that the FDTD-GSTC method requires much less number of grids and computing resources.

### Table 1: Coefficients of the four terms in complex-conjugate pole-residue pairs to fit $\chi^{xx}_{ee} = \chi^{xx}_{ee}$ for the graphene sheet with cross elements $(d = 4.13e^{-8})$

<table>
<thead>
<tr>
<th>Coefficients</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(a_{p1}\cdot c_{p1})$</td>
<td>$(-1.769\times10^3 + 0j, 9.376\times10^4 + 0j)$</td>
</tr>
<tr>
<td>$(a_{p2}\cdot c_{p2})$</td>
<td>$(-1.099\times10^3 + 0j, -4.041\times10^4 + 0j)$</td>
</tr>
<tr>
<td>$(a_{p3}\cdot c_{p3})$</td>
<td>$(-2.866\times10^3 + 0j, 1.911\times10^4 + 0j)$</td>
</tr>
<tr>
<td>$(a_{p4}\cdot c_{p4})$</td>
<td>$(-6.685\times10^3 + 6.217\times10^3 j, -5.575\times10^4 - 3.724\times10^5 j)$</td>
</tr>
</tbody>
</table>

### Table 2: Comparison of time and memory between FDTD and FDTD-GSTC

<table>
<thead>
<tr>
<th></th>
<th>FDTD</th>
<th>FDTD-GSTC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Size of Grid</td>
<td>1x1</td>
<td>2x2</td>
</tr>
<tr>
<td>Time (s)</td>
<td>208</td>
<td>27.9</td>
</tr>
<tr>
<td>Memory (MB)</td>
<td>80</td>
<td>31</td>
</tr>
</tbody>
</table>

(B) graphene with asymmetrical elements

Secondly, the graphene with asymmetrical rectangular elements as inset in Fig. 4 (c) is simulated. The dimensions of the graphene element are $30\text{um} \times 18\text{um}$, the period is $30\text{um}$. The incident modulated Gaussian pulse is with normal propagation direction and $\hat{x}$ polarization. The scattering rate of graphene sheet is 0.96meV, the temperature is 300 K, and biasing electric field on graphene is of $E = 0V/nm$.

With the complex-conjugate pole-residue pairs method, the broadband (0.5 THz to 4 THz) susceptibilities $\chi^{xx}_{ee}$ and $\chi^{xx}_{ee}$ with respect to frequencies can be fitted well as shown in Figs. 4 (a) and (b). The coefficients of the four terms in complex-conjugate pole-residue pairs are listed in Tables 3 and 4.

With the proposed dispersive FDTD-GSTC, the mesh size can be $dx = dy = dz = 1\text{um}$, which is much larger than conventional FDTD method [14], [15]. The incident modulated Gaussian pulse is with normal propagation direction, Fig. 3 (c) plots the simulated reflection coefficient the proposed dispersive FDTD-GSTC method and commercial software HFSS, very good agreement can be found.

### Table 3: Coefficients of the four terms in complex-conjugate pole-residue pairs to fit $\chi^{xx}_{ee}$ for the graphene sheet with rectangular elements $(d_1 = 2.94e^{-8})$

<table>
<thead>
<tr>
<th>Coefficients</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(a_{p1}\cdot c_{p1})$</td>
<td>$(-3.172\times10^3 + 0j, 5.008\times10^4 + 0j)$</td>
</tr>
<tr>
<td>$(a_{p2}\cdot c_{p2})$</td>
<td>$(-2.927\times10^3 + 0j, -5.269\times10^4 + 0j)$</td>
</tr>
<tr>
<td>$(a_{p3}\cdot c_{p3})$</td>
<td>$(-5.9568\times10^3 + 0j, 4.524\times10^4 + 0j)$</td>
</tr>
<tr>
<td>$(a_{p4}\cdot c_{p4})$</td>
<td>$(-1.141\times10^4 + 0j, -2.555\times10^5 + 0j)$</td>
</tr>
<tr>
<td>$(a_{p5}\cdot c_{p5})$</td>
<td>$(-2.833\times10^5 + 3.344\times10^6 j, -4.153\times10^4 - 1.291\times10^5 j)$</td>
</tr>
</tbody>
</table>
Table 4: Coefficients of the four terms in complex-conjugate pole-residue pairs to fit $\tilde{Z}_{\text{ee}}$ for the graphene sheet with rectangular elements ($d_y = 1.81 \text{e}^{-8}$)

<table>
<thead>
<tr>
<th>Coefficients</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(a_{p1}, c_{p1})$</td>
<td>$(-2.341 \times 10^4 + 0j, 3.359 \times 10^4 + 0j)$</td>
</tr>
<tr>
<td>$(a_{p2}, c_{p2})$</td>
<td>$(-5.157 \times 10^2 + 0j, -4.629 \times 10^2 + 0j)$</td>
</tr>
<tr>
<td>$(a_{p3}, c_{p3})$</td>
<td>$(-1.0758 \times 10^3 + 0j, -2.017 \times 10^2 + 0j)$</td>
</tr>
<tr>
<td>$(a_{p4}, c_{p4})$</td>
<td>$(-1.045 \times 10^2 + 4.771 \times 10^2 j, 2.147 \times 10^{-2} - 8.132 \times 10^2 j)$</td>
</tr>
<tr>
<td>$(a_{p5}, c_{p5})$</td>
<td>$(-9.357 \times 10^3 + 8.878 \times 10^3 j, 1.112 \times 10^8 + 2.161 \times 10^8 j)$</td>
</tr>
</tbody>
</table>

C graphene sheet with different biasing electric fields

Thirdly, the graphene sheets with cross elements as in Section IV-A with different biasing electric fields are simulated in this part. The graphene sheet is located on the substrate with thickness of 2um and relative dielectric constant of 2.

As shown in Figs. 5 (a)-(c), the extracting susceptibilities ($\chi_{xx} = \tilde{Z}_{xx}$) for the graphene sheet with biasing electrostatic field of 2 V/nm, 10 V/nm, and 20 V/nm are plotted, very good agreement between the fit and original data can be found. With the increase of static bias electric field, the peaks of reflection coefficient also gradually increase and shift to the high frequency regime as in Fig. 5 (d).

D turntable graphene sheet array

The last simulation example is a finite size graphene sheet composed of 10x10 cross elements as in Fig. 6. The observed frequencies are chosen at which the largest reflection occur, e.g., 0.9 THz, 1.18 THz, and 1.5 THz, respectively. The bistatic RCS is calculated by FDTD-GSTC and HFSS. It can be found that the results of the proposed method are in good agreement with the commercial software, while our proposed method is much more efficient as listed in Table 5.

![Fig. 4. Simulation of asymmetrical graphene sheet with rectangular elements: (a) extracted susceptibility $\tilde{Z}_{ee}$, (b) extracted susceptibility $\tilde{Z}_{ee}$, and (c) reflection coefficient by commercial software and proposed FDTD-GSTC method.](image-url)
Fig. 5. Simulation of the graphene sheet with different biasing electric field: (a) susceptibilities when $E = 2\text{V/nm}$, (b) susceptibilities when $E = 10\text{V/nm}$, (c) susceptibilities when $E = 20\text{V/nm}$, and (d) reflection coefficients with different static biasing electric fields.

Fig. 6. Validation: bistatic RCS of finite graphene sheet composed of $10 \times 10$ cross computed by HFSS (solid line) and FDTD-GSTC (dotted line).

Table 5: Comparison of time and memory between HFSS and FDTD-GSTC

<table>
<thead>
<tr>
<th>Method</th>
<th>Number of Elements</th>
<th>Time (hh:mm:ss)</th>
<th>Memory (GB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HFSS</td>
<td>7290500</td>
<td>38:51:39</td>
<td>32</td>
</tr>
<tr>
<td>FDTD-GSTC</td>
<td>$398\times398\times99$</td>
<td>07:49:51</td>
<td>12</td>
</tr>
</tbody>
</table>

V. CONCLUSION

We proposed an effective dispersive FDTD-GSTC method to analyze the electromagnetic property of graphene by using the complex-conjugate pole-residue pairs. Typical tunable graphene sheets with cross and rectangular elements are simulated in a broadband. The accuracy of the method and the computation performance is validated with respect to commercial software.

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