Electromagnetics Simulation of Graphene

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Graphene is a planar monoatomic layer of carbon bonded in a hexagonal structure. Recently, graphene has gained significant interest due to its potential in enabling new technologies and addressing key technological challenges. Numerous applications of graphene in a wide spectral range (from microwave to X-rays) have recognized it as a versatile material and an enabling technology. In many of these applications, electromagnetic (EM) properties of graphene are of interest. The EM properties of graphene and its related applications can be understood by means of EM simulation of graphene.

Graphene layer is extremely thin physically and also extremely thin electrically (the layer is one atom thick). This means that the thickness of a graphene layer is orders of magnitude smaller than the electromagnetic wavelengths. This feature makes modeling graphene distinctly challenging. Several works have recently been published on EM modeling of graphene. Some of them used commercial CAD software packages for this purpose and propose techniques which can be used to adapt CAD software to the special feature of graphene. The other works propose methods for modeling graphene by means of computational electromagnetics methods such as finite-difference time-domain method, method of moment, etc. Comparing these two methodologies, the former is easier to use but the latter is more efficient.

In this tutorial, we will: 1) introduce the EM properties of graphene, 2) review the methods used for EM modeling of graphene, and 3) facilitate a discussion on the effectiveness, advantages and disadvantages of the numerical methods available to model graphene. We will also discuss application of commercial software packages for EM simulation of graphene.

Keywords: computational electromagnetics, graphene, thin conductive layers
Vahid Nayyeri was born in Tehran, Iran, in 1983. He received the B.Sc. degree from the Iran University of Science and Technology (IUST), Tehran, Iran, in 2006, the M.Sc. degree from the University of Teheran, Tehran, Iran, in 2008, and the Ph.D. degree from the IUST in 2013, all in electrical engineering.

From 2007 to 2010, he worked as an RF-Circuit Designer at the IUST Research Center. He then was the technical manager of three research and industrial projects at the Antenna Research Laboratory of IUST. In Jun 2012 he joined the University of Waterloo as a Visiting Scholar. Presently, he is an assistant professor in the School of New Technologies, Iran University of Science and Technologies, Tehran, Iran. He has authored and coauthored one book (in Persian) and over 20 journal and conference technical papers. His research interests include applied and computational electromagnetics (especially the finite-difference time-domain method).

In 2014, Dr. Nayyeri received the "Distinguished Ph.D. Thesis Award" from the IEEE Iran Section for his research on the modeling of complex media and boundaries in the finite-difference time-domain method. He has served as a reviewer to several journals including the IEEE TRANSACTIONS ON ANTENNAS AND PROPAGATION, IEEE TRANSACTIONS ON MICROWAVE THEORY AND TECHNIQUES, and IEEE TRANSACTIONS ON ELECTROMAGNETIC COMPATIBILITY.

Omar M. Ramahi was born in Jerusalem, Palestine. He received the BS degrees in Mathematics and Electrical and Computer Engineering (summa cum laude) from Oregon State University, Corvallis, OR. He received the Ph.D. degree in Electrical and Computer Engineering from the University of Illinois at Urbana-Champaign under the supervision of Prof. Raj Mittra.

He held post-doctoral and visiting fellowship positions at the University of Illinois at Urbana-Champaign under the supervision of Professors Y. T. Lo and Raj Mittra. He then worked at Digital Equipment Corporation (presently, HP), where he was a member of the Alpha Server Product Development Group. In 2000, he joined the faculty of the James Clark School of Engineering at the University of Maryland at College Park as an Assistant Professor, and later as a tenured Associate Professor. At Maryland he was also a faculty member of the CALCE Electronic Products and Systems Center. Presently, he is a Professor in the Electrical and Computer Engineering Department, University of Waterloo, Ontario, Canada. He holds cross appointments with the Department of Mechanical and Mechatronics Engineering and the Department of Physics and Astronomy. He has authored and co-authored over 300 journal and conference technical papers on topics related to the electromagnetic phenomena and computational techniques to understand the same. He is a co-author of the book EMI/EMC Computational Modeling Handbook, (first edition: Kluwer, 1998, Second Ed: Springer-Verlag, 2001. Japanese edition published in 2005).

Prof. Ramahi is the winner of the 1994 Digital Equipment Corporation Cash Award, the 2004 University of Maryland Pi Tau Sigma Purple Cam Shaft Award for teaching, the Excellent Paper Award in the 2004 International Symposium on Electromagnetic Compatibility, Sendai, Japan, and the 2010 University of Waterloo Award for Excellence in Graduate Supervision. In 2012, he received the IEEE Electromagnetic Compatibility Society Technical Achievement Award.

Prof. Ramahi served as a consultant to several companies and was a co-founder of EMS-PLUS, LLC and Applied Electromagnetic Technology, LLC, and the Eastern Rugs and Gifts Company. Dr. Ramahi is an elected IEEE Fellow. In 2009, he served as a Co-Guest Editor for the Journal of Applied Physics A Special Issue on Metamaterials and Photonics. From 2009-2011, He served as IEEE EMC Society Distinguished Lecturer. Presently, he is serving as an Associate Editor for the IEEE TRANSACTIONS ON COMPONENTS, PACKAGING AND MANUFACTURING TECHNOLOGY.
ELECTROMAGNETICS
SIMULATION OF GRAPHENE

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Introduction to graphene

Electromagnetic model of graphene

How to model graphene in EM Simulations? Challenges and solutions. Advantages and disadvantages of each technique.

EM Simulation of graphene using commercial CAD packages
Introduction
- Single layer of graphite
- A planar monoatomic layer of carbon bonded in a hexagonal structure.
- Each carbon atom has one free electron

Molecular structure of graphene

High resolution transmission electron microscope images of graphene
Versatile Material

• **The strongest material**: 200 times stronger than structural steel!
• **The best electric conductor**: resistivity of the graphene sheet is less than that of silver!
• **The best heat conductor**: thermal conductivity of graphene is greater than copper, silver and diamond!
• **Almost completely transparent** (97.7% transmission of white light), yet so dense that not even helium, the smallest gas atom, can pass through it!
EM Applications

EM surface wave and **transformation optics**

*Vakil and Engheta, Science 332.6035 (2011): 1291-1294*
Optical modulator

Optical polarizer

EM Applications

Tunable infrared plasmonic devices

Electromagnetic Model
The physical thickness of graphene is around 0.1 nm. It could be modeled as an infinitesimally-thin, two-sided surface characterized by a surface conductivity.

\[
\sigma_g (\omega, \mu_c, \Gamma, T) = \frac{-je^2 k_B T}{\pi \hbar^2 (\omega - j2\Gamma)} \left[ \frac{\mu_c}{k_B T} + 2 \ln \left( \exp \left\{ -\frac{\mu_c}{k_B T} \right\} + 1 \right) \right] - \frac{je^2}{4\pi \hbar} \ln \left( \frac{2|\mu_c| - (\omega - j2\Gamma) \hbar}{2|\mu_c| + (\omega - j2\Gamma) \hbar} \right)
\]

**Intra-band Term:**
Drude like expression \( \frac{\sigma_0}{1 - j\tau \omega} \)
Dominant term for \( \omega << 2\mu_c /\hbar \)
(till low THz region)

**Inter-band Term:**
- Complex expression
- Dominant term from \( \omega \approx 2\mu_c /\hbar \)
Conductivity of Graphene

Intraband Contribution

\[ \nabla \times H = j \omega \left( \varepsilon + \frac{\sigma}{j \omega} \right) E \]

\[ \text{Im}[\sigma] \equiv \text{Re}[\varepsilon] \]
• Graphene conductivity is tunable by adjusting chemical potential $\mu_c$ which can be controlled by either an applied electrostatic bias or doping.

$$
\sigma_g(\omega, \mu_c, \Gamma, T) = \frac{-je^2k_B T}{\pi\hbar^2(\omega - j2 \Gamma)} \left[ \frac{\mu_c}{k_B T} + 2 \ln \left( \exp \left\{ -\frac{\mu_c}{k_B T} \right\} + 1 \right) \right] - \frac{je^2}{4\pi\hbar} \ln \left( \frac{2|\mu_c| - (\omega - j2 \Gamma)\hbar}{2|\mu_c| + (\omega - j2 \Gamma)\hbar} \right)
$$
Conductivity of Graphene

- For a magnetostatic biased graphene sheet, surface conductivity is in tensor form:

\[
\bar{\sigma} = \begin{bmatrix}
\sigma_d & \sigma_o \\
-\sigma_o & \sigma_d
\end{bmatrix}
\]

\[
\sigma_d = \sigma_d(\omega, \mu_c, B_0)
\]

\[
\sigma_o = \sigma_o(\omega, \mu_c, B_0)
\]

- Graphene can rotate the polarization of a linearly polarized wave
Electromagnetic Simulation
For EM simulation of graphene, we need to model graphene in computational EM methods.

There are two problems for such a purpose:

1. **Complex conductivity of graphene.**
   - *Problem in time-domain methods.*

2. **Modeling an infinitesimally-thin conductive (with finite conductivity) layer in CEM methods.**
Approximation of Conductivity

- Interband term of conductivity has a complex form (in terms of frequency) which cannot be directly implemented in a time-domain method.

- Rational functions are easily implemented in time-domain methods

- Complex conductivity of graphene can be approximation by sum of partial fractions:

\[
\sigma_g(\omega) \approx \sigma_\infty + \sum_{k=1}^{N} \sigma_k(\omega), \quad \sigma_k(\omega) = \begin{cases} 
\frac{r_k}{j\omega - p_k}; & p_k \text{ and } r_k \text{ are real} \\
\frac{r_k}{j\omega - p_k} + \frac{r_k^*}{j\omega - p_k^*}; & p_k \text{ and } r_k \text{ are complex}
\end{cases}
\]

✓ \sigma_\infty, r_k \text{ and } p_k \text{ are obtained using curve fitting or vector fitting techniques}
Accurate Approximation

\[ \mu_c = 65 \text{meV} \]

\[ \mu_c = 150 \text{meV} \]

<table>
<thead>
<tr>
<th>( k )</th>
<th>( p_k \times 10^{-14} )</th>
<th>( r_k \times 10^{-18} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,2</td>
<td>-0.4549 ± j1.8648</td>
<td>-1.2684 ± j2.6891</td>
</tr>
<tr>
<td>3,4</td>
<td>-0.0199 ± j1.6234</td>
<td>9.8688 ± j0.7526</td>
</tr>
<tr>
<td>5,6</td>
<td>-0.9675 ± j1.2734</td>
<td>-4.6157 ± j3.2365</td>
</tr>
<tr>
<td>7</td>
<td>-1.3870</td>
<td>-7.9723</td>
</tr>
</tbody>
</table>

\[ \mu_c = 150 \text{meV} \]

\[ \mu_c = 65 \text{meV} \]

\[ \times 10^{-1} \]

Frequency [THz]

Kubo formula

Approximation

18
Graphene is modeled as an infinitesimally thin (2D) conductive layer with a surface conductivity.

Surface conductivity fundamentally means a boundary condition at two sides of the sheet.

\[
\hat{n} \times \left( \mathbf{E}_2 - \mathbf{E}_1 \right) = J_s = \sigma_s E_t
\]
Applying conductive sheet boundary condition (CSBC) in the MoM (the method of moments) and the boundary element method (BEM) is straightforward.

For many problems, BEM and MoM are significantly less efficient than volume-discretization methods (finite element method, finite difference method, finite volume method).

Applying conductive sheet boundary condition in volume-discretization methods is not straightforward. Conductive sheet boundary condition is not compatible with Yee’s lattice.
Alternative Technique: Volumetric Implementation

- The easiest way is to consider graphene as a thin layer with an assumed non-zero thickness $\Delta$.
- Then, the surface conductivity of graphene should be converted to volumetric conductivity

$$\sigma_v = \frac{\sigma_s}{\Delta}$$
Alternative Technique: Volumetric Implementation

- The conductivity of graphene sheet is in-plane, so the out of plane conductivity is set to zero:

\[
\sigma_v = \begin{bmatrix}
\sigma_s/\Delta & 0 & 0 \\
0 & \sigma_s/\Delta & 0 \\
0 & 0 & 0
\end{bmatrix}
\]

\[
\sigma_{v,biased} = \begin{bmatrix}
\sigma_d/\Delta & \sigma_0/\Delta & 0 \\
-\sigma_0/\Delta & \sigma_d/\Delta & 0 \\
0 & 0 & 0
\end{bmatrix}
\]
Alternative Technique: Volumetric Implementation

- **Advantage:** very easy to implement and strikingly compatible with all volume-discretization methods and commercial software.
  - Due the above advantage, this technique has frequently been used in literature.

- **Disadvantage:**
  - To have accurate results, volumetric layer must be very thin; hence, extremely fine mesh is required. In conditional stable time domain methods, finer spatial grid needs finer time steps.
Alternative Technique: Volumetric Implementation

Check convergence as a function of thickness

Dashed black line: Results of the surface impedance model obtained by the MoM.
Solid colored lines: Results of the equivalent slab model (thickness of 500, 200, 5nm)
Alternative Technique: Volumetric Implementation

Check convergence as a function of thickness

Simulated normal-incidence transmission spectra with different grating periods. 
\[ dx=0.25\text{nm}, \ dy=0.05\text{nm}, \ \mu_c=0.64\text{eV} \]

Commonly \( \Delta \) is set to 0.3 – 5 nm
In the literature

Implementation and Application of Resistive Sheet Boundary Condition in the Finite-Difference Time-Domain Method

Lin-Kun Wu, Member, IEEE, and Liang-Tung Han

Abstract—Use of resistive sheet boundary condition in the finite-difference time-domain (FDTD) analysis of scattering problems involving a coated dielectric object is described. The algorithm is introduced through an analysis of $E$-polarized scattering from a thin resistive strip. For the sheet

In the following, the analysis technique is first derived for a two-dimensional $E$-polarized scattering problem of a thin resistive strip. The numerical stability issue of the method is also discussed. The FDTD technique is validated by compar-
Direct Implementation of CSBC

- Implementation of conductive sheet boundary condition in the FDTD method:

$$\frac{\partial B}{\partial t} = -\nabla \times E$$

\[ \frac{\partial}{\partial z}: \text{Backward and Forward Difference} \]

\[ \mu_1 \frac{H^{n+\frac{1}{2}}_x - H^{n-\frac{1}{2}}_x}{\Delta t} = \frac{E^n_y (K + \frac{1}{2}) - E^n_y (K)}{\Delta z}, \]

\[ \mu_2 \frac{H^{n+\frac{1}{2}}_x - H^{n-\frac{1}{2}}_x}{\Delta t} = \frac{E^n_y (K + 1) - E^n_y (K + \frac{1}{2})}{\Delta z}, \]

Not defined in the FDTD mesh
Direct Implementation of CSBC

- Implementation of conductive sheet boundary condition in the FDTD method:

\[ \frac{\partial B}{\partial t} = -\nabla \times E \]

\[ \frac{\partial}{\partial z} \frac{\partial B}{\partial t} = \nabla \cdot E \]

\[ \frac{1}{\mu_1} \left( \frac{H_{x}^{n+\frac{1}{2}} - H_{x}^{n-\frac{1}{2}}}{\Delta t} \right) = \frac{E_{y}^{n} (K + \frac{1}{2}) - E_{y}^{n} (K)}{\Delta z}, \]

\[ \frac{1}{\mu_2} \left( \frac{H_{x}^{n+\frac{1}{2}} - H_{x}^{n-\frac{1}{2}}}{\Delta t} \right) = \frac{E_{y}^{n} (K + 1) - E_{y}^{n} (K + \frac{1}{2})}{\Delta z}, \]

Substituted by CSBC:

\[ E_{y} = \frac{1}{\sigma_s} \left( \frac{E_{x}^{n} - E_{x}^{n-1}}{\Delta t} \right) \]
Direct Implementation of BC

- 3D Cell

Direct Implementation of BC

- Implementation of Graphene in the FEM using impedance boundary conditions

Equivalent circuit of graphene single layer

Impedance network boundary conditions

Direct Implementation of BC

Graphene ribbon: $W = 1 \mu m$, $P = 2 \mu m$

$|E|^2$: SIO$_2$ substrate, TE Polarization

$|H|^2$: TE Polarization
Transmission of the graphene micro-ribbon array for TE and TM polarized incident waves.
**Advantage**: Graphene is modeled as zero-thickness sheet. Hence the size of the mesh can be chosen independently.

**Disadvantage**: Modification on original FDTD or FEM method is required.
1. Complex conductivity of graphene.
   - Problem in time-domain methods we can approximate the conductivity by sum of partial fractions

2. Modeling an infinitesimally-thin conductive (with finite conductivity) layer in Volume-discretization CEM methods.
   - Model graphene as thin volumetric conductive layer
   - Modify the method to be compatible with conductive sheet boundary condition
Simulation using commercial EM solver
MoM frequency domain solver

The graphene sheet can be modeled as a zero-thickness resistive sheet (impedance surface).

No embedded model for graphene sheet

The surface resistivity of sheet \((1/\sigma)\) is given in a lookup table.

Unable to model magnetostatically biased graphene sheet (with anisotropic surface conductivity)
Modeling by Commercial Software

- Variables
  - c0 = 1/sqrt(eps0*mu0)
  - eps0 = 8.85418781761e-12
  - mu0 = pi*4e-7
  - pi = 3.14159265358979323846
  - z0 = sqrt(eps0*mu0)

- Named points

- Workplanes
  - Global XY [Default]
  - Global XZ
  - Global YZ

- Media
  - Perfect electric conductor
  - Perfect magnetic conductor
  - Free space

- Geometry
  - Rectangle1

- Solution
  - Infinite planes
  - Loads
  - Excitations
  - Calculation

- Optimisation

Create impedance sheet

- Manually define medium
- Import medium from file

Surface impedance (Ohm)

Definition method: Specify points (linear interpolation)

![Graph of surface impedance](image)

<table>
<thead>
<tr>
<th>Frequency</th>
<th>Real</th>
<th>Imaginary</th>
</tr>
</thead>
<tbody>
<tr>
<td>Point 1</td>
<td>f1</td>
<td>R1</td>
</tr>
<tr>
<td>Point 2</td>
<td>f2</td>
<td>R2</td>
</tr>
<tr>
<td>Point 3</td>
<td>f3</td>
<td>R3</td>
</tr>
<tr>
<td>Point 4</td>
<td>f4</td>
<td>R4</td>
</tr>
</tbody>
</table>

Label: Graphene

![Error message](image)
- Finite Integral Method (FIM) Solver in both time and frequency domain
- **There are two ways to model graphene sheet:**

  1. *The graphene sheet can be modeled as a thin volumetric layer* (the thickness of the layer is usually set to 1-3 nm). To have accurate results, the out-plane conductivity can be chosen close to zero.

  2. *The graphene sheet can be model as a surface resistive sheet* (in CST 2013 and letter)
Volumetric implementation of graphene in CST

The partial fraction approximation might be done by either user or the solver.
CST seems to be capable to model magnetostatically biased graphene sheet (with full anisotropic conductivity) as a thin layer
Implementation of graphene using Surface impedance in CST

The surface resistivity of sheet \((1/\sigma)\) is given in a lookup table.
Congratulations!
In the most recent version of CST (2014), graphene model is embedded!
Congratulations!
In the most recent version of CST (2014), graphene model is embedded!
Lumerical FDTD solution is most common software package used for simulation of graphene.

The graphene sheet is modeled as a thin volumetric layer (the thickness of the layer is usually set to 0.3-2 nm).

Lumerical has embedded graphene model in its material data-base

Capable to model magnetostatically biased graphene sheet
Modeling by Commercial Software

**Material Properties**

<table>
<thead>
<tr>
<th>Anisotropy</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>xx</td>
<td>yy</td>
</tr>
<tr>
<td>Real</td>
<td>x6 - x1 * 2 * x3 * x1 / (pi * x2^2) / (w^2 - ((x1 * x4^2) / (x5 * x3 * x1))^2) * w / (x8 * w * x7)</td>
<td>2.5</td>
</tr>
<tr>
<td>Imaginary</td>
<td>x1^2 * x3 * x1 / (pi * x2^2) / (w^2 - ((x1 * x4^2) / (x5 * x3 * x1))^2) * ((x1 * x4^2) / (x5 * x3 * x1)) / (x8 * w * x7)</td>
<td>0</td>
</tr>
</tbody>
</table>

- **Length units**: m
- **Frequency units**: Hz
- **Number of samples**: 50
- **x1**: $e$ (elementary charge)
- **x2**: $\hbar$ (reduced Planck constant)
- **x3**: $\mu_c$ (Chemical potential)
- **x4**: $v_f$ (Fermi velocity)
- **x5**: $\mu$ (mobility)
- **x6**: $\varepsilon_r$
- **x7**: $\Delta$ (graphene thickness)
- **x8**: $\varepsilon_0$ (carrier relaxation time)
 References

• Hanson, George W. "Dyadic Green’s functions and guided surface waves for a surface conductivity model of graphene." Journal of Applied Physics 103.6 (2008): 064302.
• CST Studio Suite (http://www.cst.com)
• FEKO - EM Simulation Software (https://www.feko.info/)
• Lumercial FDTD Solutions (https://www.lumerical.com/)
Thank you for your attention

Questions?

Fez, Morocco