The Multiphysics Solution to Maxwell-Hydrodynamic Equations for Modeling Terahertz Generation from Plasmonic Metasurfaces

Ming Fang¹, Zhi-Xiang Huang¹, Wei E. I. Sha²*, and Xianliang Wu¹

1. Anhui University
2. Zhejiang University

Email: weisha@zju.edu.cn (W.E.I. Sha)
Website: http://www.isee.zju.edu.cn/weisha/
Outline

• 1. Introduction
• 2. Numerical Model and Implementation
• 3. Benchmark
• 4. Broadband Terahertz Generation from Metasurface
• 5. Conclusion
• 6. Outlook
Broadband Terahertz (THz) Spectroscopy

‘THz gap’

Overview of THz Sources and Detectors

<table>
<thead>
<tr>
<th>Generation</th>
<th>Detection</th>
</tr>
</thead>
</table>
| **Electronic** | - Schottky diode  
- Backward diode  
- Rectifying transistor (Tera-FET) |
| **Laser** | - Quantum cascade laser  
- p-type Germanium laser  
- Molecule gas laser  
- Free electron laser |
| **Optical** | - Photoconductive switch antenna/photomixer  
- Optical rectification  
- Surface emitter  
- Photo-induced plasma |

### Generation of THz Waves

<table>
<thead>
<tr>
<th>Method</th>
<th>Quantum Cascade Laser</th>
<th>Photoconductive Antenna</th>
<th>Semiconductor</th>
<th>Optical Rectification</th>
<th>Electro-optical Sampling</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Schematic</strong></td>
<td><img src="image1.png" alt="Schematic" /></td>
<td><img src="image2.png" alt="Schematic" /></td>
<td><img src="image3.png" alt="Schematic" /></td>
<td><img src="image4.png" alt="Schematic" /></td>
<td><img src="image5.png" alt="Schematic" /></td>
</tr>
</tbody>
</table>

**Limited by:**
1. Excitation source (bandwidth and center frequency)
2. Operating temperature
3. Phase matching condition
4. Longitudinal optical phonon absorption
5. Defect and impurity
6. Weak nonlinear conversion efficiency
Nonlinear Plasmonics

Ref: Opt. Express 15: 5238-5247

Ref: Science 333: 1720-1723

Physical Review B 95: 165432, 2017

Scientific Reports 6: 18872, 2016

Physical Review A 83: 043824, 2011
FDTD Implementation of Maxwell-Hydrodynamic Model

Maxwell’s Equations

\[ \nabla \times \mathbf{H} = \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} + \frac{\partial \mathbf{P}}{\partial t} \]
\[ \nabla \times \mathbf{E} = -\mu_0 \frac{\partial \mathbf{H}}{\partial t}, \]

Weakly Coupled by:

\[ \frac{\partial n}{\partial t} = -\nabla \cdot (nv), \]
\[ \frac{\partial P}{\partial t} = -env. \]

Hydrodynamic Model

\[ \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{e}{m} (\mathbf{E} + \mu_0 \mathbf{v} \times \mathbf{H}) - \gamma \mathbf{v} - \frac{\nabla P}{n}. \]

The equations are solved by FDTD method with Yee grids.
Charge Conservation

At each point, the electron density fluctuates. However, the total charge within the sphere is conserved.
Energy Conservation/Conversion

\[ E_{SHG}(2\omega) \sim |E(\omega)|^2 \]

\[ E_{THG}(3\omega) \sim |E(\omega)|^3 \]
Angular Momentum Conservation (1)

n fold rotational symmetry and m\(^{th}\) harmonics

\[ \vec{E}_\sigma = \vec{E}_0 \hat{e}_\sigma = \vec{E}_0 (\hat{e}_x + i \sigma \hat{e}_y) / \sqrt{2} \]

- \( m = (n \ell - 1) \): opposite circular polarization
- \( m = (n \ell + 1) \): same circular polarization

\[ \vec{p}_{\text{pol},\sigma} = 0 \quad \text{if} \quad (m - 1)/n \text{ is not integer} \]
\[ \vec{p}_{\text{pol},-\sigma} = 0 \quad \text{if} \quad (m + 1)/n \text{ is not integer} \]
Angular Momentum Conservation (2)

Discretization of Hydrodynamic Equation

\[
v_{x}^{i+1}(i, j+1/2, k+1/2) = v_{x}^{i}(i, j+1/2, k+1/2) - \Delta t \gamma v_{x}^{i}(i, j+1/2, k+1/2) - \frac{\Delta t}{m} E_{x}^{i+1/2}(i, j+1/2, k+1/2)
\]

spatial interpolation is adopted to force all the physical quantities to be the same locations. The interpolation scheme is crucial to maintain the angular momentum conservation of nonlinear process in metals.
Broadband Metasurface THz Emitter: Experiments in Literature

Numerical Results of Metasurface THz Emitter by Maxwell-Hydrodynamic (M-H) Model

Terahertz Spectrum — Metasurface Generation and ZnTe Crystal Detection

\[ E^{(THz)}(\omega) \sim \chi^{(2)}(-i\omega)^2 g \frac{1}{\sqrt{2\sigma}} (\omega) = \chi^{(2)} \omega^2 e^{-\frac{\omega^2}{4\sigma^2}} \Rightarrow. \]

\[ E^{(THz)}(t) \sim -\chi^{(2)} \partial_t g \sqrt{2\sigma} (t) = \chi^{(2)} \sigma^2 (1-2\sigma^2 t^2)e^{-\sigma^2 t^2} \]
Tunable THz Spectrum by Duration Time or FWHM of Incident Laser Pulse

M. Fang, W.E.I. Sha, et al. Optics Express, 26(11): 14241, 2018
Incident Angle and Polarization Dependent THz Generation
Conclusion

1. A time-domain implementation of Maxwell-hydrodynamic model for conduction electrons in metals has been developed to enable nonperturbative studies of nonlinear coherent interaction between light and plasmonic nanostructures.

2. Numerical method was validated by conservation and conversion laws.

3. We numerically demonstrated a new concept of THz emitter based on a single-layer nonlinear metasurface of nanoscale thickness, representing a new platform for revealing artificial magnetism-induced THz generation.
Outlook

Maxwell’s Equations

\[ \nabla \times \mathbf{H} = \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} + \frac{\partial \mathbf{P}}{\partial t}, \]

\[ \nabla \times \mathbf{E} = -\mu_0 \frac{\partial \mathbf{H}}{\partial t}, \]

Hydrodynamic Model

\[ m n \frac{\partial n}{\partial t} + \mathbf{v} \cdot \nabla n = -n \nabla \frac{\delta G}{\delta n} + n e (\mathbf{E} + \mathbf{v} \times \mathbf{B}), \]

\[ \frac{\partial n}{\partial t} = -\nabla \cdot (n \mathbf{v}) \]

Quantum Corrections

\[ \frac{\delta G}{\delta n} = \frac{\delta T}{\delta n} + \frac{\delta F_{xc}}{\delta n} = \frac{\delta T_T}{\delta n} + \frac{\delta T_W}{\delta n} + \frac{\delta E_x}{\delta n} + \frac{\delta E_c}{\delta n} + \frac{\delta E_{LB94}}{\delta n} \]