Efficient Multiphysics and Multiscale FDTD Methods for Terahertz Plasmonic Devices

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***Abstract*—Modeling terahertz plasmonic devices is a multiphysics and multiscale problem. Due to high mesh density in the electron transport regions, the simulation times are long. In this work, we develop hybrid coupled finite difference time domain (FDTD) methods for fast design of terahertz plasmonic devices. The methods employ implicit solution (using Alternate Direction Implicit), coupled with hydrodynamic modeling for plasmonic applications. The theory, simulation and time-improvement related results will be presented at the conference.**

Keywords*—*FDTD, graphene, HEMT, hydrodynamic, plasmonic modeling, terahertz.

I. INTRODUCTION

2D electron-gas based terahertz electronics has gained interest for terahertz operations such as mixing and detection. Underlying phenomenon in these devices is plasma-wave oscillations in the 2D electron gas (2DEG) channel [1]. These 2DEG based devices can be modeled using multiphysics modeling tool that integrates the electromagnetic propagation effects and electron transport effects within the devices [2]. This is often accomplished using finite difference time domain (FDTD) based coupled models that integrate hydrodynamic equations in their solution.

A typical 2DEG-channel has an electron density of 10^{11} to $10^{13} cm^{-2}$. Therefore, the plasmonic wavelengths would be 10 to 1000 times smaller than that the free-space. This requires a mesh-size in the order of $\lambda/5000$. As per Courant-Friedrich-Levy (CFL) condition, FDTD time-step for this simulation is 10^{-17}s. This results in long simulations times using traditional FDTD coupled hydrodynamic equations.

In this work, the time-efficiency of the traditional FDTD based model [2] is improved using unconditionally stable FDTD algorithms. First, we present Alternating Direction Implicit (ADI) FDTD method [3] coupled with hydrodynamic equations for terahertz plasmonic applications. Secondly, an iterative-ADI based FDTD method [4] coupled with hydrodynamic equations, is presented for efficient yet accurate modeling. These methods are referred to as ADI-FDTD-HD and it-ADI-FDTD-HD, respectively.

II. GOVERNING EQUATIONS FOR MULTIPHYSICS MODELING

Solution requires modeling of electrodynamic fields via:

$$\nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J} + \sigma \vec{E}, \quad \text{and} \tag{1}$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} - \sigma^* \vec{H}. \tag{2}$$

For 2D TE$_Z$ solution, electric field $\vec{E} = \hat{x}E_x + \hat{y}E_y$ is used. Electrical and magnetic conductivity parameters, i.e., σ and σ^*, are used for the modeling of anisotropic, perfectly matched layer surrounding the domain. Electron transport in the channel is modelled via hydrodynamic equations, given by,

$$\frac{\partial n_{sh}}{\partial t} + \frac{\partial j}{\partial x} = 0, \quad \text{and} \tag{3}$$

$$\frac{\partial j}{\partial t} + v\frac{\partial j}{\partial x} + \frac{j\partial v}{\partial x} = -\frac{qnE_x}{m_e} - \frac{j}{\tau} - \frac{KT}{m_e}. \tag{4}$$

Here n_{sh} is the sheet carrier density, j (= $n_{sh}v$) is the sheet current and v is the electron velocity within the 2DEG channel. τ refers to the momentum relaxation time and m_e is the effective electron mass. q = 1.6×10−19 C is the charge-magnitude of a single electron. T is the electron temperature in the channel and K is the Boltzmann constant.

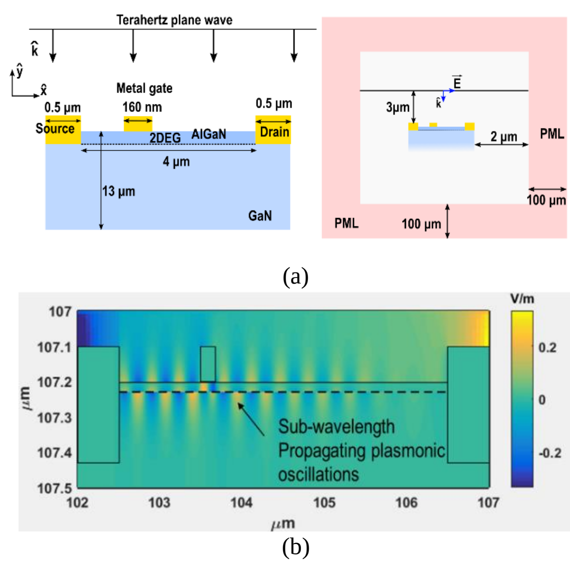

Fig. 1. GaN/AlGaN High Electron Mobility Transistor (HEMT) model used for the performance evaluation of the algorithms. Left: Schematic showing device-dimensions and excitation-method. Right: Simulation domain and position of PML boundaries. (b) Plasmonic field obtained at t=3ps, propagating away from discontinuity.

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III. ADI-FDTD-HD AND IT-ADI-FDTD-HD METHODS

Note that solution of hydrodynamic equations is carried by upwind discretization, similar to prior work in [2] and will not be discussed here. The distinction of this work, use of ADI-FDTD and it-ADI-FDTD methods, is briefly explained in the following.

A. ADI-FDTD-HD Method

The ADI-FDTD approach uses a splitting-operator applied on the electrodynamic equations to yield an implicit form of difference equations [3, 4]. Notably, these equations are tridiagonal and can be solved at a small computational cost. In the meantime, the time-steps can be arbitrarily large, reducing the simulation-times. In ADI-FDTD method, the accuracy is perturbed by a second order terms (which is truncated so as to achieve a tridiagonal system of linear implicit equations [5]). This error term (so-called splitting error or truncation error) is proportional to Δt^2 and second order spacial derivative of field [3] (Δt is the time-step).

B. Iterative ADI-FDTD-HD Method

The iterative method uses the basic ADI-FDTD method with added iterative corrections to correct ignored Δt^2 term [4]. Note that it-ADI-FDTD and ADI-FDTD are both O(Δt^2) accurate. However, iterative method has more accuracy due to correction of additionally truncated term of the ADI method. The added iterations come at some time-cost, but overall performance is maintained over the traditional FDTD-HD method.

IV. PERFORMANCE COMPARISON

For performance bench-marking, we modeled a gallium nitride (GaN) based High Electron Mobility Transistor (HEMT) device under the influence of an incident terahertz plane-wave excitation (freq. = 5 THz) (Fig. 1). A small gate discontinuity is used for coupling of the incident terahertz waves to the 2DEG channel. The channel and media parameters are chosen as $n_{sh} = 5 \times 10^{12}\, cm^{-2}$, $\epsilon_r = 9.5$, $m_e = 0.2 m_o$ and τ= 1.14 ps (considering low temperature operation). The cell-size along x-axis was chosen to be Δx = 4 nm in the channel area. The minimum mesh of Δy =1 nm was used in vertical direction. For outside the channel regions, non-uniform meshing scheme was used, resulting in 1460 and 740 cells respectively in the horizontal and vertical directions. Simulation is allowed to run for 3 ps.

For comparison, the obtained channel-currents are plotted in Fig. 2. The simulation-cases considered here are *CN*=300, <*CN*=300, *it*=3>, <*CN*=300, *it*=7>. Here *CN* refers to Courant Number and *it* refers to the number of iterations used for the iterative case. That is, *CN*=300 case is for ADI-FDTD-HD algorithm and rest are for it-ADI-FDT-HD method. As shown in the plot, in ADI-FDTD-HD method the solution diverges from the reference data, however errors are recovered by adding more and more iterations. Specifically, for 7 iterations the solution converges to the reference solution. Here, the reference solution corresponds to the Yee's FDTD method [6]. Comparison of total simulation times for various scenarios are shown in Table I. As shown *CN*=300, *it*=7 case takes only half of total simulation time taken by the original reference case. Thus, high degree of accuracy if achieved with almost 50% decrease in simulation times. Note that CPU-time for ADI-FDTD-HD cases may also be calculated by simply dividing the it-ADI-FDTD-HD's CPU time by corresponding *it* count. A more rigorous analysis and results are can be referred from [7].

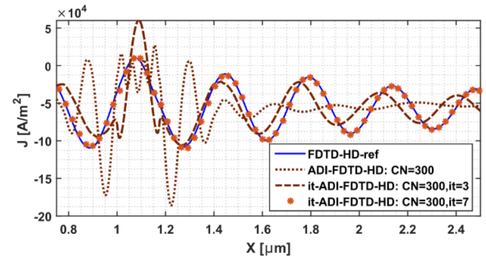

Fig. 2. Channel current at 3 ps calculated using reference (FDTD-HD) and proposed ADI-FDTD and it-ADI-FDTD schemes.

Table I. TIME COMPARISON FOR IT-ADI-FDTD-HD METHODS

`	ΔT (s)	CPU-Time Per Time-Step (s)	CPU-Time Total (Hrs)
FDTD-HD	3.24×10^{-18}	0.35	90
it-ADI-FDTD-HD (*CN*=100, *it*=2)	3.24×10^{-16}	15.17	39.14
it-ADI-FDTD-HD (*CN*=200, *it*=4)	6.48×10^{-16}	30.25	19.16
it-ADI-FDTD-HD (*CN*=300, *it*=7)	9.72×10^{-16}	53.11	43.64

V. CONCLUSIONS

We have proposed efficient method for multiphysics modeling using iterative-ADI-FDTD methods. For the devices under consideration, the total simulation time was reduced by a factor of 0.42 using it-ADI-FDTD-HD method, while nominal 3% error was registered. Overall, we maintained the accuracy-levels with significant time-cost advantages as compared to traditional explicit-FDTD modeling.

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