On The Development of A New Multi-Physics Solver for Atomically Thin Layered Material Systems

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***Abstract*—In the last decade, we have experienced a fascinating transformation in the research and development of atomically thin-layered material (ATLM) systems. Graphene and its compounds have enabled the development of novel devices for a wide variety of applications in an extremely short period of time. In addition, non-graphene ATLMs have recently been utilized to produce devices with exceptional performances. It is anticipated that ATLMs will play a crucial role in the integration of nano electronics with photonics and plasmonics in the coming decades. However, there are many challenges that need to be addressed before it is possible to convert the potential of ATLMs into reality. Their accurate and efficient modeling is one of these challenges. In this work, I briefly discuss our recent efforts on the development of a hybrid Schrödinger-Poisson and Maxwell's Equations solver that will enable us exploring how light interacts with ATLM systems in different configurations and under different biasing conditions.**

I. Introduction

The discovery of graphene [1] can be considered a revolutionary point in the research and development of stable ATLM systems. This one-atom-thick fabric of carbon uniquely combines extreme mechanical strength, exceptionally high electronic and thermal conductivities, impermeability to gases, as well as many other supreme properties making it a highly attractive material for numerous applications [2]. This breakthrough has opened up the possibility of isolating and exploring the fascinating properties of atomic layers of several other materials, which could potentially offer functional flexibility, new properties, and novel applications. Some of the material systems where preliminary work has already been released include nitrides, dichalcogenides, and oxides.

Apart from the chemical and material analyses, scientists and engineers have been using different approaches to analyze ATLM systems. For electronic applications, numerical Schrödinger-Poisson solvers have been used to characterize ATLM devices (by calculating current-voltage curves) [3]. Since graphene's electronic properties are described by the Dirac rather than Schrödinger equation, it is very common to use electrostatics or lumped-element circuit modeling to analyze graphene based devices (e.g. graphene loaded plasmonic antennas [4]). To demonstrate this approach, a grounded graphene layer on a substrate of SiO_2 and Si will be used as the example device. Voltage is applied across the Si and graphene layers creating what may be viewed as a simple parallel plate capacitor. In such a structure, the capacitance per unit area is equal to $C_g = d_{SiO_2}/\epsilon_{SiO_2}$, where d_{SiO_2} and ϵ_{SiO_2} are thickness and permittivity of SiO_2. The Fermi energy (E_F) - gate voltage (V) relationship is calculated using $E_F = \hbar v_F \sqrt{C_g V/e}$, where v_F is the Fermi velocity of graphene. This approach works very well as long as the thickness of the dielectric material (e.g. SiO_2) is very small compared to the wavelength and the geometries are simple.

For photonic and plasmonic applications, numerical Maxwell equations solvers have been used to mimic the wave propagation through and scattering from such structures [5], [6]. There are many commercial software packages (e.g. HFSS, CST, RSoft, Comsol, Feko, Wavenology, Lumerical etc.) that can be used for such analyses. These solvers use different methods and all of them have some advantages and disadvantages depending on the problem under examination. However, none of these solvers have been developed specifically for ATLM devices and this creates a big efficiency problem. For example, consider an electro-optic modulator which is fabricated on top of a graphene coated SiO_2-Si substrate. Assume the modulator operates at the telecom wavelength ($\lambda = 1550$ nm). Typical thickness values for graphene, SiO_2, and Si layers are 0.34 nm ($\lambda/4500$), 300 nm ($\lambda/5.17$), 1 mm (645 λ), respectively. Such geometry has two issues from the computational point of view: (i) some layers are extremely thick compared to the wavelength, and (ii) there is a huge variation in the layer thicknesses. The former issue requires millions of unknowns in order to take each layer into account, whereas the latter requires either domain decomposition or a denser mesh compared to a case where the thicknesses are close to each other. This is why ATLM device modeling is a very challenging task and requires its own solvers.

Another issue is the absence of a model for extremely thin surfaces. Due to the nature of their formulation, it is not possible to define a dispersive surface in time domain methods. This is why ATLM analysis should be done in the frequency domain. However, most of the frequency domain software packages do not allow us to define ATLMs (It could be that

developers believed 2D materials were not realistic or perhaps they just wanted to avoid additional computational complexity in their algorithms). Some (e.g. HFSS and CST) allow us to define ATLMs as long as we know that material's surface resistance. This puts additional computational and materialistic burden on the user, who does not have to know how to calculate the surface resistance. Special boundary conditions might be applied in FEM based frequency domain solvers (e.g. in COMSOL), however this approach is not efficient from the computational point of view due to FEM's requirement to include the whole device in the computation domain.

Another problem with commercial electromagnetic software packages is an inability to calculate the gate voltage required to change the Fermi energy (E_F) of the ATLM to the desired level. For complex structures, we cannot determine what will happen if we apply 5 volts of gate voltage or how much voltage we need to apply to change E_F to 0.5 eV.

II. A Hybrid Schrödinger-Poisson and Maxwell's Equations Solver

In order to overcome these problems, we propose to hybridize Schrödinger-Poisson and Maxwell's Equations solvers as follows. Assume we would like to analyze a plasmonic waveguide placed on top of an ATLM coated substrate, as shown in Fig. 1.

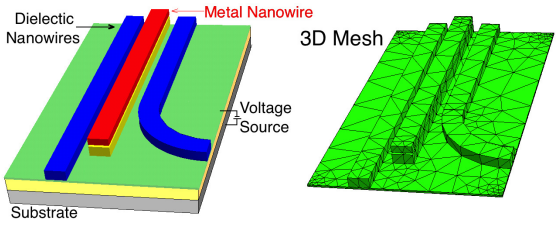

Fig. 1. (a) A plasmonic waveguide placed on top of an ATLM coated substrate and (b) meshed volume to be used in a hybrid volume-surface integral equation solver

In order to take quantum effects into account, we first use Quantum3D, which is a commercial Schrödinger-Poisson (SP) equation solver by assuming a trial gate potential and solve for SP equation to calculate carrier density and currents from the obtained wave-functions and their corresponding eigen-energies. Then, the obtained carrier density and currents are input to a hybrid volume-surface integral equation solver and calculate fields and potentials. If the final potential is bigger (smaller) than the initial guess, we go back to the first step with a bigger (smaller) trial gate potential. We iterate until we satisfy $|V_{initial} - V_{final}| < \delta V_{final}$, where δ is a very small number (e.g. $\delta = 10^{-4}$). By solving both Schrödinger-Poisson and Maxwell equations simultaneously, it is expected to understand gate voltage - Fermi level energy relationship of the ATLM under examination.

We have two different hybrid Maxwell Equation solvers. One of them is a hybrid MoM/FEM solver [11]–[13], which assumes a homogeneous background. Other one is implemented with layered medium Green's functions to handle multi-layered structures [7]–[11]. However, in order to couple these SP and Maxwell's equations solvers, the hybrid volume-surface integral equations matrix should be modified. For example, all the edges taken on the ATLM, a special boundary condition $(\Delta(\hat{\mathbf{n}} \cdot \mathbf{H}) + 4\pi\sigma_{ATLM}(\hat{\mathbf{n}} \times \mathbf{E})/c = 0)$ has to be enforced, where σ_{ATLM} is the two-dimensional conductivity of the ATLM. It should be noted that σ_{ATLM} changes when the applied voltage changes. Gate voltage - conductivity relation for graphene can be found in [14]. Our preliminary studies show that using a two-dimensional conductivity for the modeling of an ATLM increases computational efficiency compared to the case where the ATLM is modeled with an effective complex electrical permittivity and a finite thickness [15]. At the conference, we will discuss our preliminary results and the advantages of formulating the Maxwell solver with layered medium Green's functions.

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