3D Model of Terahertz Photoconductive Antenna usign COMSOL Multiphysics

Jose Santos and Magda El-Shenawee
University of Arkansas
Fayetteville, AR, United States
jisantos@uark.edu, magda@uark.edu

***Abstract*—This paper presents a 3D model of a photoconductive antenna (PCA) on semiconductor substrate. The simulations were conducted using the COMSOL Multiphysics package. The model considers the laser excitation and the carrier generation acceleration in the semiconductor layer. The computational work was achieved using the frequency-domain RF module and the semiconductor module. The results demonstrate that simulating the active area alone produces sufficient accuracy ~ 0.01% in the RF module solution (solution of the electric and magnetic fields) and ~ 0.23% in the semiconductor solution (photocurrent solution). The reduction in the simulated area helps minimizing the required CPU time and memory requirement in the 3D model at THz frequencies. The largest case in this study was simulated at the National XSEDE Supercomputing with ~ 0.3 billion unknowns and memory requirement of ~ 3.2TB in the RF module.**

Keywords—terahertz; photoconductive antenna; computational requirements; model reduction

I. Introduction

Terahertz photoconductive antenna (PCA) emitters are devices capable of transforming a femtosecond laser pulse into time-domain pulse that carries frequency components in the terahertz (THz) range [1]. The structure of a conventional PCA emitter consists of a semiconductor substrate with electrodes deposited on its surface and separated by a gap, where the femtosecond laser is focused. Conventional PCAs have been in the literature for a long time, and researchers have been focused on improving its performance based in terms of optical-to-terahertz efficiency and bandwidth [1]. To provide performance improvements to these devices, it is important to develop accurate models that contribute to the understanding of its functioning. With this goal, this work presents some considerations and challenges for a three-dimensional (3D) model of the PCA performance including its femtosecond laser excitation and carrier dynamics in the semiconductor layer. A 3D model improves the accuracy of the results compared to a model in two dimensions (2D) as it includes more features such as the distribution of the laser source in both x- and y-direction as well as the actual shape of the electrodes.

II. Methodology

The commercial package COMSOL Multiphysics was used to simulate the performance of a photoconductive antenna emitter. Due to the extensive computational requirements of a 3D model at high frequency, our local AHPCC and the National XSEDE Supercomputing Centers were unutilized for the simulations presented in this work. To simulate models in the high-performance computing center, the Floating Network License (FNL) of COMSOL Multiphysics was required. This license allows the simulation in multiple nodes, which resembles the computer structure of the high-performance computing center.

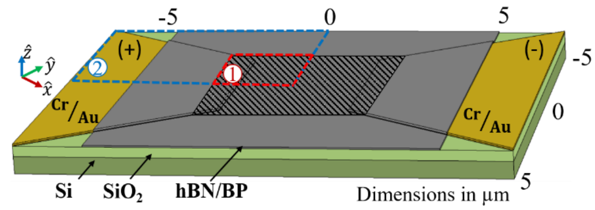

Fig. 1. Device geometry configuration and modeling domain description for the RF module and semiconductor module solution [4].

The modeled photoconductive antenna is presented for two different semiconductor materials: the conventional LT-GaAs in 2D/3D model [3] and the new material black phosphorus (BP) [4]. The later material has anisotropic crystal structure that presents high optical absorption, high mobility, and saturation velocity [2]. The geometry configurations of the modeled devices (LT-GaAs and BP) are similar in principal but different in details. In Fig. 1, we show the geometry of a BP PCA where the semiconductor layer is positioned in the gap of the antenna covered by a layer of hexagonal boron nitride (hBN) [3]. The substrate is composed of a layer of SiO_2 and half space of Si. The thicknesses of these layers were taken from [4], which presented a 3D computational model for the performance of a PCA emitter. The model consists of three parts: optical, electrical, and terahertz responses. This paper is focused on modeling considerations applicable to the first two parts.

The optical response represents the modeling of the femtosecond laser excitation and its interaction with the multilayer device. Due to the fine wavelength-depended ($\lambda/10$) discretization required for the solution of Maxwell's equation and the dimensions of the antenna in micrometer scale, modeling the laser excitation was computationally expensive problem. To overcome the computational domain challenge, only the active area of the device was modeled as reported by [5]. The active area is the region close to the gap, where the laser is focused, and is shown by the shaded square in Fig. 1. In addition. to reduce the modeling domain more, the perfect electric conductor (PEC) and perfect magnetic conductor (PMC) boundary conditions were applied to exploit the symmetry of the device geometry. In this way, only one quarter of the active area was simulated as shown by the red-dashed square in Fig. 1. Using the electric and magnetic fields solutions obtain in this quarter, the maximum power density in the semiconductor was calculated [4]. This maximum power density is considered the source excitation for the electrical response of the device, which consists of modeling the carrier generation and the acceleration of those carriers due to the application of the bias voltage to the electrodes. The modeling domain is shown in Fig. 1, where the electrical response only considered the BP layer. The material properties for both optical and electrical response were reported in [4].

III. Results and Discussion

The results of the optical response of this model is shown in Fig. 2 for both case ① and case ② shown in Fig. 1. Case ① was solved using the AHPCC, and case ② was solved using XSEDE. These plots represents the electric field at any point in the computational domain. The solution presented in Fig. 2(a) represents the electric field solution of the dashed square in Fig. 1, which covers one quarter of the active area. In the same way, the results presented in Fig. 2(b) shows the electric field solution for one quarter of a larger domain than the active area. The purpose of this study is to demonstrate that modeling the active area of the device is sufficiently accurate compared with modeling a larger domain. Upon comparison of both cases, we report a difference of ~ 0.01% between both solutions in agreement with [5].

In terms of the electrical response, the same comparison was conducted. The electrical response of the larger case ② marked in Fig. 1 was simulated and compared against the electrical response of the active area marked by ①. The results are shown in Fig. 3, where the simulation of only the active area in Fig. 3(a) showed similar photocurrent values compared to Fig. 3(b). Both solutions presented higher photocurrent density at the electrodes edges which is the result of edge effect in the solution of the bias electric field. However, the edges of the electrodes in Fig. 3(b) showed photocurrent density over a wider space. Fig. 3(c) showed the photocurrent comparison obtained at a single point at 10 nm below the surface of the BP layer at the center of the gap. From this plot, the difference between both cases is shown to be ~ 0.23 % at the peak of the photocurrent density. Solving the electrical response of only the active area of the PCA produces significantly accurate results compared simulating a larger domain.

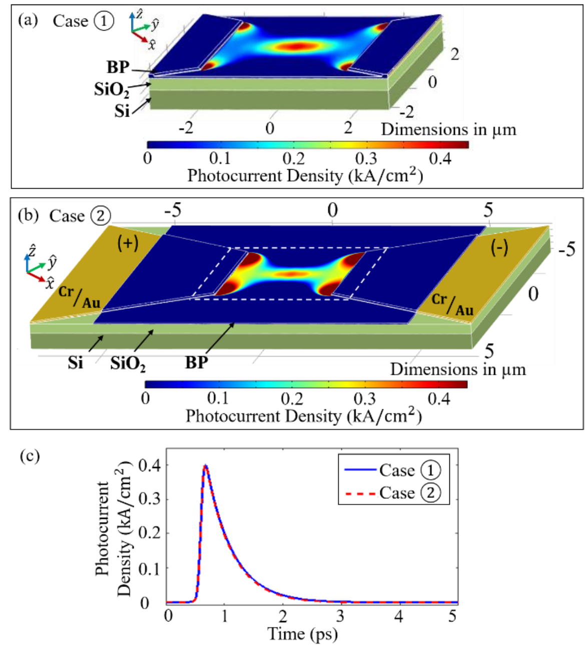

Fig. 3. Electrical response solution of a BP PCA by solving (a) the active area only compared to (b) the solution of a larger domain. (c) Photocurrent density comparison between the active area and a larger domain.

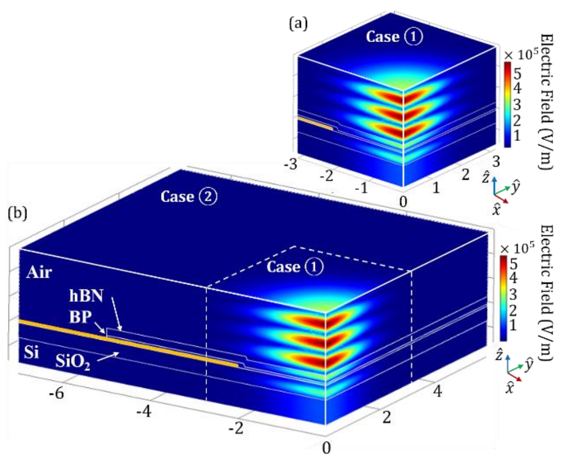

Fig. 2. Electric field from the optical response solution of the device geometry shown in Fig. 1 for (a) Case ① and (b) Case ②

IV. Conclusion

The studies presented in this work demonstrated that solving the electrical and optical responses of only the active area of a PCA provides sufficiently accurate results compared to solving a larger domain. In fact, the percentage difference experienced for the optical response was ~ 0.01% and 0.23% for the electrical response at the peak of the photocurrent density. Simulating only the active area of the PCA leads to significant reduction in the computational cost of the solution.

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