Comparative Study of Three Wave Propagation Software Programs for the Modeling of Coupled Maxwell and Boltzmann Equations at THz Frequency

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Abstract **–** The modeling of optoelectronic devices operating at THz frequency requires self consistently solving the Maxwell equations and the Boltzmann transport equation. In this article, it is the numerical method for solving Maxwell's equations that is debated in the frame of its ability to be combined with transport equations. For this purpose, three software programs mainly devoted to the simulation of 3D electromagnetic equations in time-domain (one based on a 3D finite element method and two on 3D FDTD methods) are first presented and compared. The structure used for the modeling comparison is a coplanar waveguide structure. Results provided by the three solvers are compared according to two factors of merit. Then, the coupling of Maxwell and Boltzmann equations in the FDTD frame is briefly presented and the difficulties to use other methods are explained, showing that the variable-mesh FDTD method is most suitable for such a coupling.

I. INTRODUCTION

The behavior of a THz optoelectronic device such as a photoconductive switch excited by a fs laser pulse is controlled by the coupling between two physical phenomena: the photo-generated carrier transport and the electromagnetic propagation. The modeling of electromagnetic propagation requires to solve Maxwell's equations (the all set of equations) while for the transport of carriers supposed to be classical it is necessary to solve the Boltzmann Transport Equation (BTE). During these last few years, we developed at the Institut d'Electronique Fondamentale (IEF) a software (MAXTRA3D) to solve the whole equation system (Maxwell equations and carrier transport equations) [1]. The software is based on a 3D Finite-Difference Time-Domain (FDTD) method with a variable step mesh allowing a realistic structure design for an accurate description of photo-generated carriers and of their transport mechanisms.

The very first question one asked at the beginning of this work consisted in finding the appropriate numerical approach to solve both electromagnetic and transport equations self consistently. The finite element methods seemed to be the best suited ones. But the modeling of electromagnetic propagation was an autonomous field of study with its dedicated methods and no method could be drawn aside a priori. The 3D electromagnetic problems in time domain can be solved by various numerical methods: FDTD [2], Transmission Line Matrix (TLM) [3], Finite Integrated Technique (FIT) [4], Finite Element Method (FEM) [5], Finite Volume (FV) [6] and Discontinuous Galerkin Methods (DGM) [7]. Among all of these methods, this article focuses on one variational method, the finite element method (FEM) and on one differential method, the FDTD method. This choice has been mainly motivated by two factors. First, FDTD is an explicit method with the capability to perform 3D realistic propagation simulation. Secondly, FEM is a powerful method for carrier transport simulation with complex geometries. Taking into account all this considerations, the best suited method for solving Maxwell equations but also for combining these equations with transport equations can be identified.

Previous works have been already done concerning hybrid full wave models. The review article by Grondin et al [3] provides a good overview of the work done in this area prior to 1999. More recently, some articles provide last development in these Topics ([9-11]). The authors present a Full Band hybrid model based on a Monte Carlo resolution of the BTE. In the most recent articles, the authors used a non uniform mesh to simulate an InGaAs HEMT (High Electron Mobility Transistor). But some progresses need also to be done to provide a

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totally self consistent Maxwell and Boltzmann solver with a non uniform meshing. Moreover some critical mechanisms such as the quantum confinement of electrons in the HEMT channel and therefore the 2D transport of electrons are not taken into account yet in these hybrid models. The topic is difficult and many works have still to be done in next future.

The article is divided into three main parts. After this introduction, three software programs mainly devoted to the simulation of 3D electromagnetic equations in time-domain are presented in the first section. A short overview of these numerical tools is provided to the readers. These tools can solve a large variety of electromagnetic phenomena but we insist here on their specificity and on their main application domain. The first software FEM from LGEP [12] is based on a finite element method and the second software TEMSI-FD from XLIM [13] is based on a 3D FDTD method with constant mesh step. To finish this section, the propagation part of the last software MAXTRA3D is introduced and a briefly overview of its application domains is given. In the second section, the results provided by the different software on a basic structure (coplanar waveguide) are compared in order to exhibit their abilities to solve accurately the propagation phenomena. The third section shows some results of coupling Maxwell and Boltzmann equations within FDTD frame with MAXTRA3D applied to a Photoconductive Switch (PS) device.

II. SOFTWARE PRESENTATION (MAXTRA3D, TEMSI-FD, FEM)

A. FDTD Method

Both TEMSI-FD and MAXTRA3D software are based on FDTD method. This numerical method allows the solution of the set of Maxwell equations in a rigorous manner. The FDTD (finite difference time domain) technique developed by K.S. Yee [2] discretizes the two Maxwell curl equations directly in time and spatial domains, and put them into iterative forms. The physical geometry is divided into small (mostly rectangular or cubical) cells. Both time and spatial partial derivatives are handled with finite central difference approximation and the solution is obtained with a leapfrog scheme in iterative form. The characteristics of the medium are defined by three parameters that are permittivity, conductivity and permeability. Three electric and three magnetic field components are calculated at different locations of each cell [14]. Beside the spatial differences in field components, there is also a half time step difference between electric and magnetic field components, which is called as leapfrog computation. The numerical stability of the common FDTD scheme is ensured by respecting the relationship between the time and the spatial steps known as CFL (Courant-Friedrichs-Levy) stability criterion [2]. Besides, when using non regular mesh FDTD, it is important to reduce the numerical dispersion by choosing an appropriate value for the greatest spatial increment. It must be smaller than λ /10, where λ is the wavelength in the medium corresponding to the highest frequency of operation (≈1 THz). This numerical method owes its success to the power and simplicity that it provides. Furthermore, it is possible to achieve the response in a chosen frequency band in one calculation by using a pulse excitation. This cannot be achieved with a frequency domain method. On the other hand the Cartesian grid conforms badly to the real geometry, thus introducing so called stair stepping errors. Besides, one disadvantage of FDTD is that, in common with most other techniques, the problem size and the thinness of the mesh will dictate the computation time. The fineness of the grid is determined by the dimensions of the smallest feature to be modeled, and so codes that offer a variation in the mesh size over the structure would have an advantage. Also, the entire object, including most of the near field, must be covered.

TEMSI-FD is a numerical code based on 3D FDTD analysis that uses a uniform mesh. It has been developed at XLIM institute to simulate wide variety of wave-matter interaction problems. It has been coded with Fortran 90 language and is suited for vector processors (like Nec-SX8) and SMP architectures (Symmetric MultiProcessing) by development of OPEN-MP parallelism. Hence billion cells can be solved efficiently from eight Nec-SX8 processors of the CNRS/IDRIS (French intensive computing center). To truncate the computational domains for open-region wave propagation problems, TEMSI-FD use the Convolution Perfect Matched Layers (CPML) that offers a number of advantages. Specifically, the application of the CPML is completely independent of the host medium. Secondly, it is shown that the CPML is highly absorption of evanescent. TEMSI-FD has already been used to simulate various technologies: ground penetrating radars [15], Wifi transmission systems [16]. More generally, the software is devoted to EMC studies [17].

MAXTRA3D is 3D FDTD code using non-uniform mesh. It is developed by IEF laboratory in order to couple the Maxwell and the transport equations to model optoelectronic devices at terahertz frequency. For a question of simplicity, the same method (an integrated approach) was chosen for both propagation and transport equations. The transport property of the carriers is simulated within the frame of a 3D Drift-Diffusion approach or of a 3D Hydrodynamic model. Both models are solved using the FDTD numeric scheme as for the Maxwell equations. These transport models provide the local current density which constitutes the source term in Maxwell equations. All the data required for the transport model namely momentum and energy relaxation times, or effective mass versus average carrier energy are calculated using a Monte-Carlo solver. When coupling a Monte-Carlo solver of the BTE with a FDTD base solver of Maxwell equations, we did observe a large variance of current density in the Monte Carlo code due to the strong variation of carrier concentration from cells below the optical pulse to the others. So the numerically determinist codes (Drift Diffusion and Hydrodynamic) were preferred instead of a stochastic solvers for the transport equation.

The current version of MAXTRA3D is numerically stable as a result of rewording of both material passages and current interfaces and calculating transport equations on whole transport region without imposing a fixed conductivity. The solver actually runs in a Dual-Core AMD Opteron with 16 GB Ram that allows the reduction of computation time as well as modular and optimal programming. The formulation used to truncate FDTD lattice in MAXTRA3D is the uniaxial anisotropic PML (UPML) introduced by S. D. Gedney [18]. This formulation has the advantage of keeping Maxwell's equations in their familiar form without the need of Berenger's field splitting. MAXTRA3D has been designed to simulate compact optoelectronic structures (Photoconductive switches). But the main goal of the software is to investigate the optoelectronic devices in conjunction with his propagation environment when operating in THz frequency.

B. Finite Element Method in Time Domain

A 3D finite element method for numerically solving the vector wave equation in time domain has been developed (FEM software) in the Laboratoire de Génie Electrique de Paris. The method uses Whitney's edge element on tetrahedral for the electric field interpolation. The time derivates are discretized by the Newmark Method, which allows an unconditionally stable scheme with second order accuracy. The finite-element time-domain method proposed by L. Pichon is mainly devoted to EMC studies [12] or antenna analysis [19]. Let's focus on the edge element approximation. The electromagnetic analysis is achieved by a finite element time domain approach. In the time domain, the electromagnetic problem is described with the double curl's equation. The studied domain is discretized with tetrahedral elements and the electric vector is written in terms of first order tetrahedral edge elements. The finite-element time-domain method provides increased geometrical flexibility by making elements conform to complex features. Furthermore, finite elements lead to irregular meshes and take easily inhomogeneous materials. The edge element method [20] can be considered as one of the most important methods developed 15 years after the FDTD method. The edge elements used in FEM preserve the energy and guarantee the continuity of the tangential field component across the interelement boundaries. The studied region in which the fields are computed must be bounded. In FEM a Silver-Müller absorbing condition (first order) was chosen because it was easy to implement and allowed us to obtain a satisfactory results [21].

The variational formulation of the electromagnetic problem described with the double curl's equation leads to an ordinary differential equation (ODE equation). In order to solve this equation step-by-step in time, the time derivates must be approximated by finite difference. We use the Newmark method. This standard approach (consistent method) leads to a high computational cost, since a matrix inversion is needed at each time step. So, there is a strong motivation to use mass-lumping technique [22] to deal with transient Maxwell's equations. In this approach, an explicit scheme is obtained allowing an important decrease in memory CPU time since no matrix inversion is required [23].

The next section is devoted to a comparison of Gaussian shape electric pulse propagation in a coplanar waveguide with MAXTRA3D, FEM and TEMSI-FD. The size of the structure has been chosen quite small because in FEM a matrix has to be invert at each time step.

III. MODELINGS

A. The Structure Selected for the Comparison

The modeled structure is a coplanar waveguide (CPW) with infinite ground planes. The length of the guide is 100µm, a width of the central band S and of the lateral ground planes is 10µm and the spacing between the central band and the ground planes W is 6µm.

The CPW is excited with two voltages placed in the ground plane surface. The electric fields of excitation are symmetrical with respect to the plane (xz), and each is placed between the central band and one of the ground planes (Fig. 1). The excitation is a Gaussian pulse with a Full Width at Half Maximum of 100 fs and maximum amplitude of 0.6 V. The next section describes the simulation environment for the different software namely the mesh and boundary condition parameters.

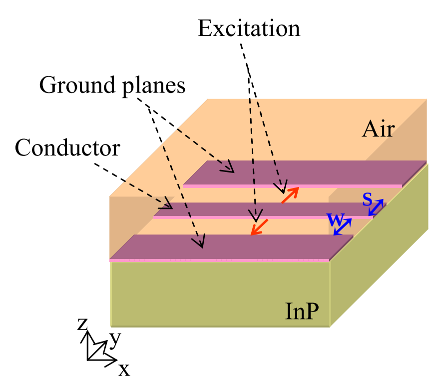


Fig. 1. CPW modeled structure.

B. Modeling Environment

Three different designs are used to mesh the CPW reference structure (Figs. 2 to 4). The first one is used by both TEMSI-FD and MAXTRA3D and it is the 1µm regular grid structure. The mesh dimensions are 100 × 62 × 100 respectively following x, y and z directions. The second one is used by MAXTRA3D and it is the variable orthogonal mesh scheme with 1 µm as the smallest mesh size and 40 × 24 × 40 mesh dimensions. The last one is used by the FEM and it is the tetrahedral finite element scheme with 1 µm as the smallest mesh size and 37128 elements (6947 nodes and 45542 edges). The time step estimated for TEMSI-FD and MAXTRA3D (with uniform or variable grid) is 1.88732fs with 2119 iterations. And for FEM, the time step is equal to 20 fs. The simulation duration chosen for all the simulations is 4 ps.

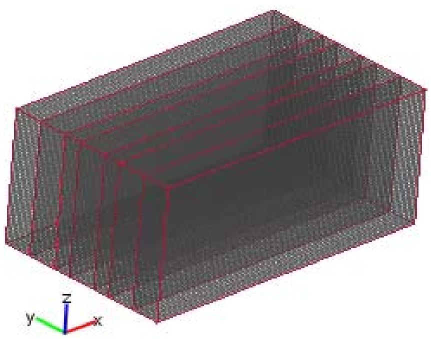


Fig. 2. Uniform mesh scheme (TEMSI-FD and MAXTRA3D).

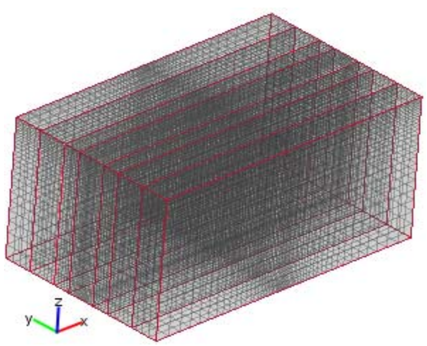


Fig. 3. Variable orthogonal mesh scheme (MAXTRA3D).

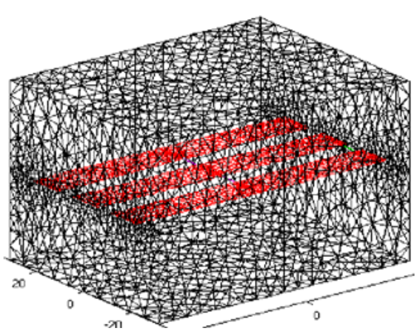


Fig. 4. Variable tetrahedral mesh scheme (FEM).

In open-region electromagnetic simulations, the computational domain has to be truncated by absorbing boundary conditions (ABC) to model the infinite space. In TEMSI-FD software, the ABC applied are Convolutional PML (CPML) conditions. In MAXTRA3D, the ABC adopted are PML and MUR conditions. And in the FEM software, the ABC are Silver-Müller conditions.

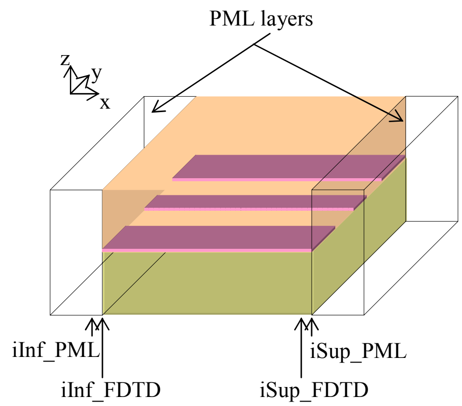


Fig. 5. PML layers added along the propagation direction.

The simulation results presented in the following section are carried out with TEMSI-FD, FEM and MAXTRA3D using the variable-mesh configuration for this last one (with MUR conditions at the first time and UPML conditions at the second time (Fig. 5)). All the FDTD simulations are running on a Dual-Core AMD Opteron with 16 GB RAM.

C. Results and Comparison

The results of calculations coming from the three software programs are obviously close but they also exhibit some differences. In order to identify those differences, we have selected two factors of merit: the amplitude error and the runtime. It is believed that the results provided by TEMSI-FD are most accurate since they are using a constant mesh (fewer numerical errors) and the most successful boundary conditions (CPML). Fig. 6 shows TEMSI-FD results of the wave propagation at three different distances from the excitation source (4 µm, 20 µm and 48 µm). One notes that the return to the equilibrium state (0 Volt) is free of any numerical oscillations contrary to the solution of Maxtra3D with MUR conditions (Fig. 7). In Fig. 8, one compares the results of the propagation at 20 µm from the excitation source for FEM, MAXTRA3D with MUR conditions and TEMSI-FD. One can notice that the result of Maxtra3D with MUR conditions have the same shape before 1 ps than TEMSI-FD result with an amplitude error of 0.015 V. However, the electric pulse shape calculated with MAXTRA3D seems to be like the one calculated with FEM. In fact, there are some oscillations before the return to the equilibrium state. In order to point up the influence of the MAXTRA3D ABC on the simulation results, we display in Fig. 9 the same results than those in Fig. 8 but we substitute MAXTRA3D result that use MUR conditions with the one using UPML conditions. We can see a right correlation between MAXTRA3D and TEMSI-FD results. table 1 shows the differences between the results of TEMSI-FD, FEM and the two configuration of MAXTRA3D (with MUR or UPML) through two factors of merit. The first factor that is the amplitude error allows us to see that the deviation between the reference results of TEMSI-FD and the other software results increases when the ABC used are MUR conditions and can reach 13% close the edge of the structure. While the deviation is significantly smaller when using UPML conditions because it takes low value around 1%. This result is not original. PML conditions are known to provide far better result than MUR conditions. In addition, the runtime that is the second factor of merit indicates that using non uniform mesh for the FDTD method reduces the runtime and divides it by three (with UPML conditions) and even by four (with MUR conditions).

Table 1. The comparison of software results by using two factors of merit: the amplitude percent error at three different distances from the excitation source and the total runtime.

Software	Amplitude Percent Error			Total Runtime
	At 4 µm	At 20 µm	At 48 µm	
FEM	7.88 %	13.2 %	15.8 %	7mn10s
MAXTRA3D -MUR-	1.98 %	3.84 %	13.29 %	1mn13s
MAXTRA3D -UPML-	1.73 %	1.85 %	1.52 %	1mn45s
TEMSI-FD	Reference results			4mn52s

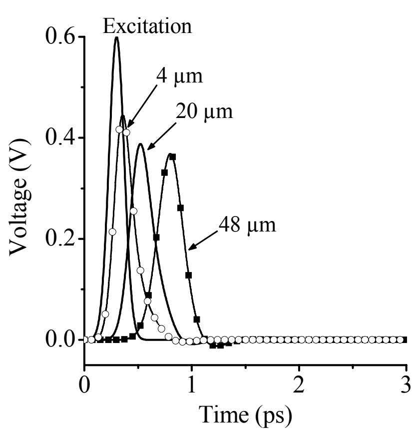


Fig. 6. Terahertz wave propagation along the CPW solved by TEMSI-FD software.

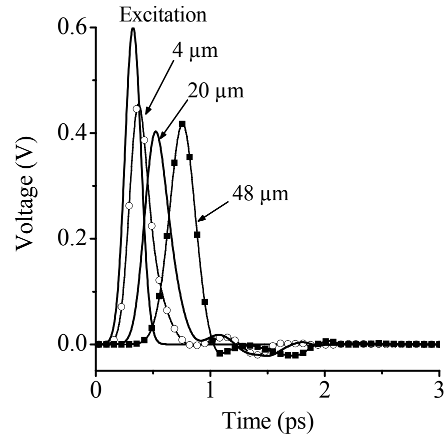


Fig. 7. Terahertz wave propagation along the CPW solved by MAXTRA3D software with MUR conditions.

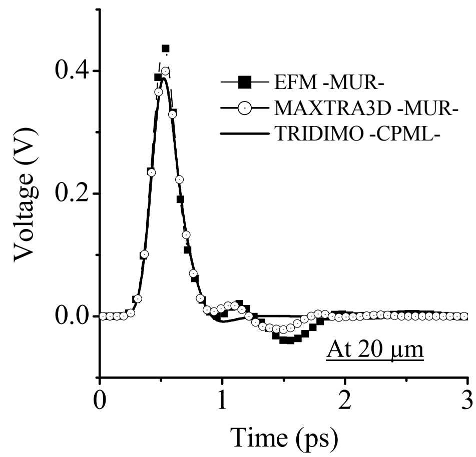


Fig. 8. The comparison of the electric pulse at 20 µm from the excitation source for the different simulators: FEM, MAXTRA3D with MUR conditions and TEMSI-FD.

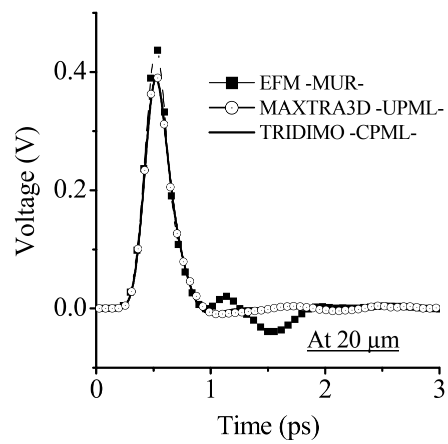


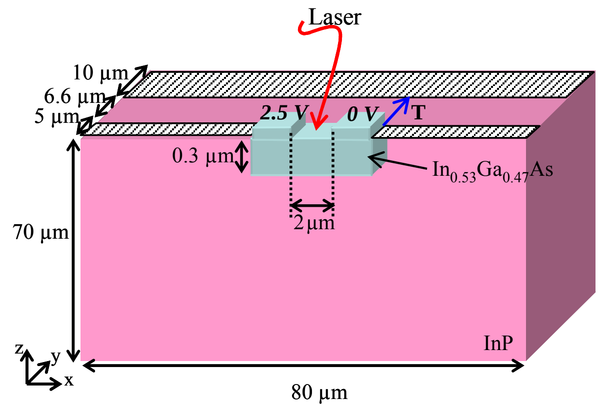
Fig. 9. The comparison of the electric pulse at 20 µm from the excitation source for the different simulators: FEM, MAXTRA3D with UPML conditions and TEMSI-FD.

IV. DISCUSSION

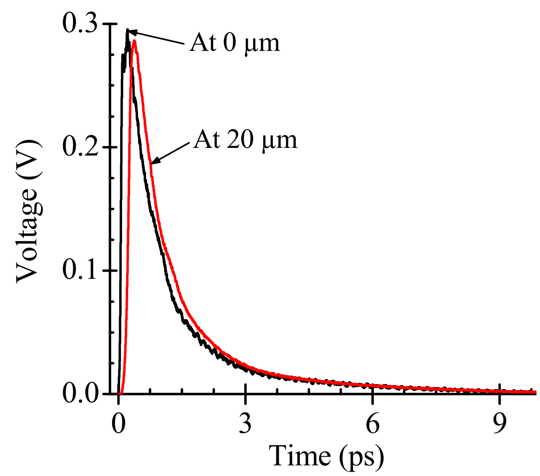
The comparison of TEMSI-FD, MAXTRA3D and FEM has been performed on a coplanar waveguide, in order to compare the three software programs only for their ability to simulate the wave propagation. TEMSI-FD, MAXTRA3D and the FEM software provide qualitatively and quantitatively almost the same results for the coplanar waveguide. The main difference is concentrated on the runtime. This is a key issue for the coupling of Maxwell equations with transport equations. MAXTRA3D has been developed for this purpose. This last paragraph is devoted to a very short discussion on the difficulties to identify a method that could be used to solve both the propagation and the transport (an integrated method). The previous results are good materials for the discussion. The FEM method has the longest runtime relatively to the FDTD method. The major weakness of finite element in time-domain comes from the presence of the mass matrix in front of the time derivative. At each time step in the Newmark scheme it is necessary to solve the linear system. The use of gradient conjugate leads to an algorithm with an O(n2) complexity if the number of unknowns is n. So the difference in runtime between the explicit FDTD method and the implicit FEM method will rapidly increase. Some authors have proposed to use a mass lumping technique [23] in order to get quasi-explicit method in time-domain like FDTD method. But even with a quasi-explicit scheme FEM methods require to manipulate matrix. The size of the matrix for the system Maxwell-Boltzmann exceeds 2 GB RAM. In the first and the second sections, the FDTD method with non uniform grid thanks to its runtime performances and its mesh fle1xibility has been identified as a good candidate for solving Maxwell equations.

These performances have been exploited to solve self consistently the Maxwell equations with Drift-Diffusion (DD) approach in a Coplanar Photoconductive Switch (PS) [1]. This coupling have already been investigated by some research teams ([3, 4, 24, 25]) but the defined spatial increment was great for the transport model because of the disproportion between the active layer size where the carrier transport happens and the environment skirting it. Here, THz voltage response of PS is briefly presented to illustrate this coupling with variable-mesh FDTD method. The details of the coupling will not be discussed here because it is not the main purpose of the present article. For more details about the coupling involving the Drift-Diffusion model one can refer to [1].

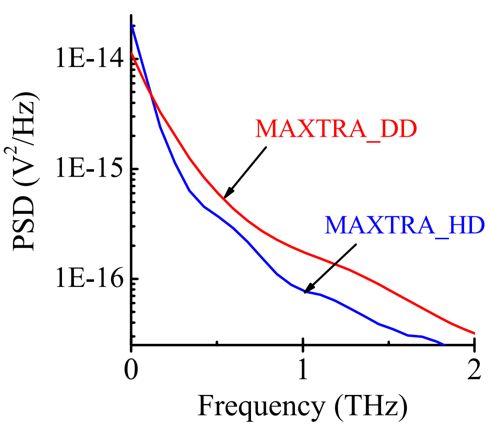
The simulated PS is described in fig. 10.a. The structure is a 2 µm broad gap in the center conductor of the waveguide. The active layer (gap) is a 0.3 µm depth In0.53Ga0.47As thin film. The CPW is the same structure as described previously at section 1 with a 76 µm depth InP substrate. A 2.5 V bias is applied between the Ohmic contacts located in CPW central strip.



(a) Cross-section of the photoconductive switch



(b) Output voltage wave at 0 µm and 20 µm at the edge of the gap with MAXTRA_DD.



(c) Output power spectral density at 20 µm calculated with MAXTRA_DD and with MAXTRA_HD model

Fig. 10. Photoconductive switch and the terahertz response.

The gap is excited by a 30 fs Gaussian shape laser pulse at 1550 nm. It is necessary to couple the electromagnetic propagation to the photo-generated carrier transports because the shape of the THz pulse is mainly controlled by the mixing of the two physics. The voltage pulse presented in Fig. 10(a) is obtained following the integration path ($\vec{T}$) drawn in the same figure between the central metallization and the ground planes. The propagation of this voltage pulse is illustrated in Fig. 10(b) and it results from the drift-diffusion & full-wave (MAXTRA_DD) coupling [1]. At the edge of the gap (0 V), the generated electric pulse rises tanks to the conduction current and falls down when the number of individual and very local conduction current source decreases in each layer. This pulse propagates along the guide (the pulse at 20 µm from the gap is presented in Fig. 10(b) with time-lag and its peak widening represents a multimode propagating in the waveguide.

The Fig. 10(c) shows the comparison of the power spectral density (PSD) propagating calculated with MAXTRA_DD and MAXTRA_HD (the hydrodynamic & full-wave code) in the coplanar waveguide at 20µm from the edge of the gap. In the Hydrodynamic modeling, the inertial effect modeled through the momentum and energy relaxation times involves a smaller frequency extension of the PSD if one compares with Drift-Diffusion modeling. The maximum amplitude and the time shape of the voltage pulse modeled by the two simulators are slightly different.

On the other hand, the FDTD method has already been compared to mixed methods (FDTD-FVM [26] and FDTD-FEM [27]). To improve the accuracy of the PS active layer modeling, some mixed approaches should be investigated. But the difficulties linked to the use of other methods (TLM, FEM, FV, FIT, DGM) with transport model is far to be simple. The main advantage of these methods in MAXTRA3D is linked to transport equations and consequently the mesh refinement. However, care should be taken at execution runtime.

V. CONCLUSION

In this article, it has been demonstrated that the variable-mesh FDTD code (Maxtra3D) is one of the most powerful technique because of its ability to combine physics required different size of meshes. When focusing on the modeling of electromagnetic problem, the results for the comparison of 3D variable-mesh FDTD method showed close agreement with those obtained both by the 3D finite element method and the 3D constant step mesh FDTD method. Moreover, Maxtra3D enables to reduce the memory storage and the computational time without degrading results. Consequently FDTD scheme is tractable to perform a coupling between electromagnetism and carrier transport physics with a much reduced step meshing when necessary. For instance, in the active layer of a PS the mesh is forty times smaller than in the peripheral access waveguide. The variable-mesh FDTD method could be used for a large number of structures requiring a meshing both at the nanometer scale and at the micrometer scale. It could be interesting to investigate in the future new mixing numerical methods for the improvement of the coupling of physics.

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