Integration of the Finite-Difference-Time-Domain and Mode-Propagation-by-Fourier-Expansion Methods for Guided-Wave Device Simulation

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ABSTRACT

A three-dimensional (3D) waveguide simulation technique is presented. The technique combines the finite-difference-time-domain (FDTD) and mode-propagation-by-Fourier-expansion (MPFE) methods for guided-wave device simulation. The algorithm consists of dividing the device into a series of small sections in which the FDTD method is employed to simulate for very complete wave characteristics. In particular, the wave characteristics around abrupt junctions of the device are simulated comprehensively by this algorithm. At the end of each section, the MPFE method is applied to simulate for optical modes and their profiles. These modes and profiles are used to extract mode parameters from the FDTD results for individual mode analysis. The modes and extracted parameters are further served as inputs to the next section for continued FDTD simulation. Thus, one can simulate arbitrarily shaped and optically large devices for very complete wave characteristics by using these two methods iteratively. The technique, together with well established semiconductor process and device simulators, presents a well-rounded methodology for semiconductor integrated-optic device simulation. This simulation methodology is illustrated by simulation and analysis of a variety of silicon based electro-optic modulators and branching waveguide structures.

1. INTRODUCTION

Analysis and simulation of electromagnetic wave propagation are essential in design and modeling of guided-wave optoelectronic devices. One of very popular methods is the finite-difference-time-domain (FDTD) method firstly introduced by Yee¹. The FDTD algorithm solves Maxwell's time-dependent curl equations in a leap-frog manner, and proceeds to obtain wave characteristics of the device. Because of the generality of the algorithm, the FDTD method can simulate for a variety of wave propagation, radiation and scattering characteristics. However, there are two inherent restrictions for the method. One is that the simulated field distribution of the wave is mixed with both guided and radiation modes. Analysis of individual mode is difficult. The other is that the FDTD simulation always requires a large amount of computer time and memory. Nonuniform gridding and a robust computer are usually required in order to simulate optically large structures^{2,3}.

Another attractive method in analysis and simulation of guided-wave devices is mode propagation by Fourier expansion (MPFE) recently introduced by Henry and Shani^{4,5}. The MPFE method consists of dividing the device into a series of sections in which optical modes are expressed by two-dimensional (2D) Fourier series. The scalar wave equation is converted into a matrix eigenvalue equation, and optical modes in each section are obtained by solving the matrix eigenvalue problem. Propagation of the modes is formulated by relating the modes and mode amplitudes of adjacent sections through coupling. This method is very efficient in simulating arbitrarily shaped and optically large devices for steady-state guided-mode propagation characteristics. The MPFE method is a time-independent algorithm and only approximates the continuum radiation field by a few discrete radiation modes.

In this paper, we combine and make use of the advantages of the FDTD and MPFE methods for analysis and simulation of guided-wave optoelectronic devices. We divide the device into a series of small sections in which the FDTD

method is firstly employed to simulate for more complete wave characteristics. In particular, wave propagation within the section is analyzed and radiation loss along the boundary is calculated. At the end of each section, the MPFE method is applied to simulate for optical modes and their profiles. These modes and profiles are used to extract mode parameters from the FDTD results for individual mode analysis. The modes and extracted parameters are further served as inputs to the next section for continued FDTD simulation. Thus, arbitrarily shaped and optically large devices can be analyzed by the FDTD method, while the results are expressed in the easily interpreted mode solution form.

The remainder of this paper is organized as follows. In Section 2, the integration the FDTD and MPFE methods is described. We refer this simulation technique as the FDTD-MPFE method. In Section 3, examples of realistic device structures are analyzed by the FDTD-MPFE method, and the simulation results are discussed. The characteristics and applications of the FDTD-MPFE method are summarized and concluded in Section 4.

2. INTEGRATION OF THE FDTD AND MPFE METHODS

Figure 1 shows a schematic diagram of wave propagation in a guided-wave device which is divided into a series of small sections. When an optical field is incident into the device, some of the incident energy is guided along the device, while the rest is absorbed or scattered away. The propagation, absorption and radiation characteristics of the wave can be simulated by the FDTD algorithm. After the simulation reaches steady state, the field distribution of the optical wave consists of a finite number of guided modes and a continuum spectrum of radiation modes. At the end of the s th section, $z = z_s$, the field distribution can be written as

$$E_{out}^s(x, y, z_s; t) = \sum_{m=1}^{N_g^s} \left(A_m^s e^{j(\omega t - k n_m^s z_s)} + B_m^s e^{j(\omega t + k n_m^s z_s)} \right) \cdot \Phi_m^s(x, y) + \int_0^\infty R^s(u; t) \cdot \Phi^s(u; x, y) du + c.c. \quad (1)$$

Where N_g^s is the total number of guided modes at the end of the s th section; A_m^s and B_m^s are the m th guided-mode amplitudes for forward and backward propagation, respectively; ω is the angular frequency; k is the wave vector; n_m^s is the m th guided-mode index; $\Phi_m^s(x, y)$ is the field distribution or mode profile of the m th guided mode; $R^s(u; t)$ is the amplitude of the radiation modes; $\Phi^s(u; x, y)$ is the field distribution of the radiation modes; and *c.c.* stands for complex conjugate. For most of the guided-wave optoelectronic devices of interests[6,7], reflected waves can always be neglected because of the adiabatic nature of the devices. Consequently, B_m^s is set to zero and the backward propagation is ignored in the formulation.

In order to determine the guided-mode amplitude A_m^s from the total field distribution $E_{out}^s(x, y, z_s; t)$, one needs to know the field distribution or mode profile of the desired guided mode $\Phi_m^s(x, y)$. The MPFE method presents one of the most efficient algorithms in determining the guided-mode index and profile for arbitrarily shaped dielectric waveguides^{4,5}. The MPFE algorithm expands the optical field in 2D Fourier series and converts the scalar wave equation into a matrix eigenvalue problem. The guided-mode index and profile can then be obtained by solving the eigenvalue problem. In the MPFE algorithm, the solved eigenvalue leads directly to the guided-mode index. While the mode profile is related to the eigenvector and basis function as follows

$$\Phi_m^s(x, y) = \sum_{j=1}^{N_M^s} a_{jm}^s \chi_j(x, y) \quad (2)$$

Where N_M^s is the total number of optical modes in the MPFE simulation, $\sum_{j=1}^{N_M^s} a_{jm}^s$ is the eigenvector of the m th mode, and

$$\chi_j(x, y) = \frac{2}{\sqrt{L_x L_y}} \sin\left(\frac{p\pi x}{L_x}\right) \sin\left(\frac{q\pi y}{L_y}\right) \quad (3)$$

is the basis function. In expression (3), L_x and L_y are the x - and y -dimensions of the box of the MPFE simulation; while p and q represent the j th basis function, or the p th x wave and q th y wave, respectively. With the mode profile obtained from the MPFE simulation, one can extract the guided-mode amplitude A_m^s from the total field distribution $E_{out}^s(x, y, z_s; t)$ by an overlap integral

$$A_m^s = \iint E_{out}^s(x, y, z_s; t) \cdot \Phi_m^s(x, y) dx dy, \quad (4)$$

where the integral is carried over the whole cross section at the end of the s th section.

Individual guided-mode analysis is now possible with the knowledge of the guided-mode index, amplitude and profile. In particular, one can evaluate optical power carried by each guided mode, one can estimate the total power guided by the device by summing up all the power carried by the guided modes, one can also distinguish the dispersion characteristics among the modes. The phase difference between the l th and m th guided modes at the end of the s th section can be approximated by the following formula

$$\Delta\phi_{lm}^s = \phi_l^s - \phi_m^s = \sum_{j=1}^s kn_l^j (z_j - z_{j-1}) - \sum_{j=1}^s kn_m^j (z_j - z_{j-1}), \quad (5)$$

where ϕ_l^s and ϕ_m^s are the optical path of the l th and m th mode at the end of the s th section, respectively.

In addition to the guided-mode analysis, radiation field distribution at the end of the section can also be extracted. This is done by subtracting all the calculated field distribution of the guided modes from the total field distribution,

$$\begin{aligned} E_{rad}^s(x, y, z_s; t) &= \int_0^\infty R^s(u; t) \cdot \Phi^s(u; x, y) du \\ &= E_{out}^s(x, y, z_s; t) - \sum_{m=1}^{N_g^s} A_m^s e^{j(\omega t - \phi_m^s)} \cdot \Phi_m^s(x, y). \end{aligned} \quad (6)$$

Thus, radiation mode can also be analyzed. The mode index and profile obtained from the MPFE simulation and the mode amplitude extracted from the FDTD results are further served as inputs to the next section for continued FDTD simulation. The input excitation for the $(s+1)$ th section can be expressed in terms of all the discrete guided modes and the continuum radiation modes at the end of the s th section as

$$E_{in}^{s+1}(x, y, z_s; t) = \sum_{m=1}^{N_g^s} A_m^s e^{j(\omega t - \phi_m^s)} \cdot \Phi_m^s(x, y) + E_{rad}^s(x, y, z_s; t). \quad (7)$$

where each guided mode has a different amplitude A_m^s and phase $\phi_m^s = \sum_{j=1}^s kn_m^j (z_j - z_{j-1})$.

One advantage of using the FDTD method for guided-wave device simulation is the generality of the algorithm. A variety of wave characteristics can be simulated. In addition to the wave propagation analysis mentioned earlier, one can also simulate for the absorption and radiation losses of the device. The absorption loss is included in the simulation through the conductivity tensor σ in the Maxwell's equations. To quantify the absorption loss, the forward propagation power at the end of the device was evaluated with and without the conductivity, respectively. The difference in the simulated power is therefore due to the absorption loss

$$P_{abs} = \int_{A_z} E \times H|_{\sigma=0} \cdot d\vec{a}_z - \int_{A_z} E \times H \cdot d\vec{a}_z. \quad (8)$$

Where E and H are the electric and magnetic field vectors, respectively; $d\vec{a}_z$ denotes the differential vector area at the end of the device and is normal to the propagation direction; and A_z is the area of the cross section at the end of the device.

To evaluate the radiation loss, one needs to integrate all the out-going power cross the boundary of the device. Therefore, it is necessary to have a very accurate boundary condition for the FDTD simulation. We used Liao's absorbing boundary condition⁸ for the FDTD simulation. Liao's absorbing boundary condition is a multi-transmitting method with which incident waves of arbitrary angles can be transmitted completely through the boundary. In the implementation of the FDTD codes, the second-order transmitting formula of Liao's algorithm was used. The error induced at the boundary was at the same order of magnitude compared with the truncation error of the finite difference computation. With the absorbing boundary condition incorporated into the algorithm, we can simulate for accurate electric and magnetic fields at the boundary. The radiation loss can then be written as the integration of all the out-going Poynting vectors over the transverse boundary of the device as follows

$$P_{rad} = \int_{A_\phi} E \times H \cdot d\vec{a}_\phi. \quad (9)$$

Where $d\vec{a}_\phi$ denotes the differential vector area along the boundary which is transverse to the propagation direction, and A_ϕ is the area of the transverse boundary of the device.

3. APPLICATIONS

By using the FDTD and MPFE methods iteratively, one can simulate arbitrarily shaped and optically large devices for a variety of wave characteristics. By further incorporating the FDTD-MPFE method with well established semiconductor process and device simulators, one can analyze and simulate semiconductor based integrated-optic devices for both optical and electrical characteristics. In the following, we apply this simulation methodology to simulate a silicon based radiation-type intensity modulator and a branching waveguide switch. These structures utilize the carrier-injection mechanism for carrier generation and the carrier-dispersion effect⁹ for electro-optic modulation.

3.1 A Radiation-type Intensity Modulator

Figure 2 shows a schematic diagram of a silicon based guided-wave electro-optic modulator. The modulator is built on a P^+/P^+ wafer where the buried 2- μm P^+ layer acts as the lower cladding and anode for the device. A channel waveguide is formed on the 4- μm P^- epi layer by anisotropic etching, whereas the lightly doped P^- layer is the core and the SiO_2 and air surrounding the core is the cladding. This channel waveguide serves as a basic building block to couple light into and out of the modulator.

The modulator has a wider dimension than the waveguide, and has a vertical $P^+-P^--N^+$ structure on each side, respectively. These two $P^+-P^--N^+$ structures are separated by a spacing equal to the width of the channel waveguide. A great amount of optical power is lost when the optical wave travels from the channel waveguide into the modulator because of the mismatch of the waveguiding characteristics at the junction. The optical wave suffers more and more radiation loss as it travels deep into the modulator since the modulator lacks of lateral confinement for the wave. However, by applying a forward bias across the $P^+-P^--N^+$ structures and injecting carriers into the P^- regions, we can decrease the refractive index in these regions and forms the lateral cladding. The wave can then be confined in the modulator, the radiation loss is reduced and an intensity modulation occurs. This structure characterizes a class of recently proposed silicon based guided-wave device structures^{10,11}, except that the latter start with silicon-on-insulator (SOI) wafers.

The device structure and doping profiles of the modulator were obtained from a SUPREM-IV¹² process simulation. Whereas, the channel waveguide was formed by anisotropic etching, and both the anodes and cathodes of the $P^+-P^--N^+$ structures were done by ion implantations. The width of the channel waveguide was 8 μm which was chosen to optimize the single-mode fiber coupling for the waveguide. This structure was used to start the electrical simulation by a semiconductor device simulator PISCES-IIB¹³. The objective of the electrical simulation is to express carrier concentration distribution of the modulator in terms of applied voltage. Modulation speed and admittance of the modulator were also examined. The simulated carrier concentration distribution was further converted to a refractive index profile by the carrier-dispersion effect⁹, which has been quantified by an empirical expression at $\lambda = 1.3 \mu\text{m}$ as

$$\Delta n = -6.2 \times 10^{-22} (\Delta N)^{1.0} - 6.0 \times 10^{-18} (\Delta P)^{0.8}, \quad (10)$$

where Δn is the refractive index, and ΔN and ΔP are the electron and hole concentration perturbations, respectively. Figure 3 shows the simulated refractive-index distribution around the modulator without bias and under a forward bias of 2 V. A waveguide with the same width of the channel waveguide within the modulator is formed when the forward bias is applied.

With the refractive index profiles obtained by the electrical simulations, one can proceed to simulate these profiles for their optical characteristics by the FDTD-MPFE method. The objective of the optical simulation is to compute mode propagation properties of the modulator and to estimate the optical modulation efficiency. the FDTD method was firstly employed to simulate for the input coupling at the input end of the waveguide. At the end of this input section, the MPFE method was applied to simulate for the steady-state optical modes and to extract mode parameters from the FDTD results. The modes and extracted mode parameters were then served as inputs for the next FDTD simulation at the waveguide-to-modulator junction. This FDTD-MPFE process was repeated within the modulator until the modulator-to-waveguide junction was reached.

In order to perform the FDTD simulation with limited computer memory, the modulator is divided into many small sections of 5 μm long. The grid spacing was uniformly 0.1 μm or $\lambda/13$ in x , y , and z directions, where the wavelength λ is 1.3 μm . As a result, the computation region in each section contained $240 \times 80 \times 50$ cells. With all six electric and magnetic

field components included in the simulation, the required memory was 56 megabytes (MB). The computation took 175 minutes or 54 cycles of input sine wave excitation to reach within 2% of the steady-state solution on a 76 MIPS HP 9000/730 machine. To further reach within 1% of the steady-state solution, it took 120 more minutes or 38 more cycles for computation. In the MPFE simulation, 24 x waves and 16 y waves were used. The computation required 3 MB memory and 7 minutes to complete on the computer.

It was found that the waveguide was able to support only one guided mode which had a mode index of 3.4923. The second higher mode had a mode index of 3.4883 which was slightly less than the lower cladding index which was 3.49. Hence, the second higher mode did not have the vertical confinement. The power carried by this mode will leak downward into the silicon substrate. The mode index difference between these two modes gives a phase difference of 4.83 *rad/mm* at $\lambda = 1.3 \mu\text{m}$. It was also found from the simulation that 64% of the optical power was coupled from the fiber to the waveguide by a direct coupling. Out of this 64% of power, 51% was carried by the fundamental mode and the rest was dispersed among other modes.

The radiation loss at the waveguide-to-modulator junction is significant when both $P^+-P^-N^+$ structures are not biased. The radiation loss is caused by the excitation of radiation modes at the junction due to imperfect coupling between the waveguide and the modulator. Because of lacking of the lateral confinement in the modulator, many horizontal radiation modes are excited at the junction. As a result, optical power is leaked away by radiation as the wave propagates through the modulator. The propagation loss consists of both the radiation and absorption losses. It was found from the simulation that most of the loss was due to the radiation. The propagation loss along the modulator without bias is shown in Figure 4.

When the modulator was forward biased, a waveguide was established within the modulator. As a result, more optical power can be confined and propagated through the modulator to the output channel waveguide. The magnitude of the confined and transmitted power depends on the degree of the lateral confinement of the modulator waveguide, which in turn depends on the concentration of the injected carriers inside the $P^+-P^-N^+$ structures. A higher forward bias can inject more carriers into the cladding P^- regions of the modulator, and results in a higher refractive-index difference between the cladding and core of the modulator waveguide. Hence, a higher confinement is reached and more light is transmitted through the modulator. Figure 5 shows the intensity modulation for the modulator at bias $V = 0$ to 2 V with respect to $V = 0$ V for a modulation length of 1 mm. The modulation started to increase when the biased exceeded 0.8 V above which carriers are heavily injected into the modulator. The intensity modulation could attain up to 35% when the bias was 2 V.

3.2 A Branching Waveguide Switch

Another interesting device is the branching waveguide switch as shown in Figure 6. The device resembles the radiation-type intensity modulator. A channel waveguide in the front is used to couple light from the fiber into the Y-branch region where there are one vertical $P^+-P^-N^+$ structure on each side, respectively. The $P^+-P^-N^+$ structures are used to control the direction of the light to the right or left. When a forward bias is applied to the right $P^+-P^-N^+$ structure, carriers are injected into its P^- region and forms a cladding. As a result, the light travelling through the Y junction will gradually turn into the right, and enter the right arm of the Y-junction. Similarly, by applying a forward bias to the left $P^+-P^-N^+$ structure, light will be reverted into the left arm. Thus, switching of light occurs.

Similar to the radiation-type intensity modulator, the simulation involves both electrical and optical simulations. For optical simulation, the computation intensive FDTD simulation is only applied to the input end of the channel waveguide and the Y-branch region. When both branches are unbiased, equal power are delivered into both arms and only negligible radiation loss is observed in the Y-branch region. However, when a forward bias is applied to one branch, a cladding is established in its P^- region. As a result, more power is switched toward the opposite arm. In addition, the power travelling through the cladding branch further suffers absorption loss due to free carriers. The split of power is determined by the refractive-index lowering in the cladding branch, or the bias applied to the branch. Figure 7 shows the split of power in both arms for the branching waveguide switch at bias from $V = 0$ to 2 V. The branching angle for the waveguide switch is 1° .

It was found from the simulation that up to 40% of optical power can be switched from one arm to the other when the bias is 2 V. At this bias, the remained power in the cladding branch is 5% and the rest 5% of power is lost by free-carrier absorption and radiation.

4. CONCLUSION

We have presented and illustrated the use of a 3D waveguide simulation technique for guided-wave device simulation. The technique combines and makes use of the advantages of the FDTD and MPFE methods, and at the same time relieves some of these method's restrictions, for guided-wave device simulation. The algorithm consists of dividing the device into a series of small sections in which the FDTD method is employed to simulate wave characteristics. The division of the device into small sections allows us to simulate very complete wave characteristics with limited computer memory. The simulation time for the whole device is also shortened. At the end of each section, the MPFE method is applied to simulate for optical modes and their profiles. These modes and profiles are used to extract mode parameters from the FDTD simulation results for individual mode analysis. The use of the MPFE method provides us a very efficient way of extracting mode characteristics from the FDTD simulation results. The field distribution of the wave obtained at the end of each section can then be expressed in terms of mode solution form. Mode propagation properties, loss mechanisms and dispersion characteristics of the wave can be easily analyzed. The modes and extracted parameters are further served as inputs to the next section for continued FDTD simulation. Thus, the device can be simulated by the FDTD method, while the results are expressed in the easily interpreted mode solution form. This technique is very useful for simulation and analysis of arbitrarily shaped and optically large adiabatic optical devices. The technique, together with the well established semiconductor process and device simulators, presents a well-rounded simulation methodology for semiconductor integrated-optic device simulation. Such as waveguide modulators, branching waveguide switch and multiplexer.

5. ACKNOWLEDGMENTS

This research was supported by a research grant awarded by the Research Grants Council under the University and Polytechnic Grants Committee of Hong Kong.

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Fig. 1 The schematical diagram of wave propagation in a guided-wave device.

Fig. 2 The schematic diagram of a silicon based guided-wave electro-optic modulator.

Fig. 3 The simulated lateral refractive-index profiles in the middle of the modulator a) without bias, and b) under a forward bias of 2 V.

Fig. 4 The propagation loss along the modulator without bias

Fig. 5 The intensity modulation of the modulator at bias $V = 0$ to 2 V with respect to $V = 0$ V

Fig. 6 The schematic diagram of a silicon based branching waveguide switch.

Fig. 7 Power split ratio in both arms for the branching waveguide at bias $V = 0$ to $2V$