Full-wave Solution of the Second Harmonic Generation Problem Using a Nonlinear FDTD Algorithm

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Abstract— A vectorial time-domain simulator of integrated optical structures containing second order nonlinearities is presented. The simulation algorithm is based on the direct solution of nonlinear Maxwell's equations representing the propagating fields and is solved using the FDTD method. Because the proposed algorithm accounts for the full optical coefficient tensor, the inaccuracies associated with the scalar and paraxial approximations are avoided. It should find application in a wide range of device structures and in the analysis of short-pulse propagation in second order nonlinear devices.

1. INTRODUCTION

The increased progress in materials technology and fabrication methods for integrated optics has resulted in a growing need for accurate models that closely predict the behavior of the electromagnetic fields inside new optical devices. Fortunately, the advent of fast and powerful computers has made detailed numerical modeling an efficient and reliable tool for researchers and engineers. Because many of the nonlinear optical devices are waveguide-based, the paraxial approximation of the energy flow direction was utilized in the early numerical models. The Beam Propagation Method (BPM) [1] is one approach of this type of modeling. The BPM method has been successfully used in the analysis of Second Harmonic Generation (SHG) in nonlinear optical structures [2, 3]. Although this method is relatively less computationally intensive than other methods, the formulation of the fields for the SHG is scalar and the method is aimed at modeling wave propagation in devices where the primary flow of energy is along a single principal direction. Other modeling methods in this area are the Finite element method (FEM) and the Finite-Difference Time-Domain (FDTD) method.

Since the introduction of the Yee algorithm for the numerical solution of Maxwell's equations in 1966 [4], the FDTD method has been applied to the simulation of a large number of linear as well as nonlinear electromagnetic problems [5]. The FDTD is substantially more robust than other methods because it directly solves for fundamental quantities. It also avoids the simplifying assumptions of conventional asymptotic behavior and paraxial propagation. Recently, a FDTD approach that solves the nonlinear scalar wave equation was applied to the second harmonic generation problem [6]. This scalar model offered a number of attractive advantages. All the effects due to the wave-medium interaction are included in the analysis under the scalar formulation. Further, as compared to the BPM solution, the approach takes into account wave reflection due to discontinuities in the simulated structure as well as outside boundaries. However, the scalar model is only suited for problems that do not involve change in polarization. In most practical nonlinear integrated optical devices, wave polarization does occur. For example, in a GaAs-based nonlinear structure a TM incident field can couple to a TE second harmonic field.

In this paper, a formulation of the full-wave model for SHG in optical structures containing second order nonlinearity is presented. This formulation is suitable for implementation using the vectorial FDTD. The algorithm is applied to a GaAs-based waveguiding structure.

2. FORMULATION OF THE SHG IN GAAS-BASED STRUCTURES

The propagation of electromagnetic radiation through certain class of crystals causes the nonlinear dielectric properties of the material to be polarized. This polarization, P, can be expressed mathematically using terms proportional to the nonlinear susceptibility, $\chi^{(2)}$, and to the propagating electric field components inside the structure. The nonlinear response of the material to such property leads to an exchange of energy between fields propagating at different frequencies. This response is utilized in the SHG in which energy from one field propagating at frequency ω_f, the fundamental field, is transferred to a field propagating at double the frequency $\omega_s = 2\omega_f$, the second harmonic field.

The formulation starts with Maxwell's equations:

$$\frac{\partial H}{\partial t} = -\frac{1}{\mu_o}\nabla \times E \tag{1}$$

$$\frac{\partial E}{\partial t} = -\frac{1}{\varepsilon_o}\nabla \times H - \frac{1}{\varepsilon_o}\frac{\partial P}{\partial t} \tag{2}$$

where E is the electric field intensity and H is the magnetic field intensity. P is the total (linear and non-linear) electric polarization given by

$$P = P^L + P^{NL} \tag{3}$$

where

$$P^L = \varepsilon_o([\varepsilon_r] - 1)E \tag{4}$$

$$P^{NL} = 2\varepsilon_o[d]E \cdot E \tag{5}$$

and $[d]$ is the nonlinear optical coefficient tensor. In vectorial form, the nonlinear polarizations of the fundamental and the second harmonic waves are given by

$$\begin{bmatrix} P_x^{NL,\omega} \\ P_y^{NL,\omega} \\ P_z^{NL,\omega} \end{bmatrix} = 2\varepsilon_o[d] \begin{bmatrix} E_x^\omega E_x^{2\omega} \\ E_y^\omega E_y^{2\omega} \\ E_z^\omega E_z^{2\omega} \\ E_z^\omega E_y^{2\omega} + E_y^\omega E_z^{2\omega} \\ E_z^\omega E_x^{2\omega} + E_x^\omega E_z^{2\omega} \\ E_x^\omega E_y^{2\omega} + E_y^\omega E_x^{2\omega} \end{bmatrix} \quad \begin{bmatrix} P_x^{NL,2\omega} \\ P_y^{NL,2\omega} \\ P_z^{NL,2\omega} \end{bmatrix} = \varepsilon_o[d] \begin{bmatrix} E_x^\omega E_x^\omega \\ E_y^\omega E_y^\omega \\ E_z^\omega E_z^\omega \\ 2E_z^\omega E_y^\omega \\ 2E_x^\omega E_z^\omega \\ 2E_x^\omega E_y^\omega \end{bmatrix} \tag{6}$$

Consider now a GaAs-based waveguide with crystal axes matching the principal axes. The nonlinear optical coefficient tensor is given by

$$[d] = \begin{bmatrix} 0 & 0 & d_{14} & 0 & 0 \\ 0 & 0 & 0 & d_{14} & 0 \\ 0 & 0 & 0 & 0 & d_{14} \end{bmatrix} \tag{7}$$

In this case, coupling of a TM fundamental field to a TE second harmonic field is possible. The resulting differential equations are:

TM fundamental input

$$\varepsilon_x \frac{\partial E_x^f}{\partial t} = -\frac{\partial H_y^f}{\partial z} - 2\varepsilon_o d_{14}\frac{\partial}{\partial t}\left(E_z^f E_y^s\right) \tag{8}$$

$$\varepsilon_z \frac{\partial E_z^f}{\partial t} = \frac{\partial H_y^f}{\partial x} - 2\varepsilon_o d_{14}\frac{\partial}{\partial t}\left(E_x^f E_y^s\right) \tag{9}$$

$$\mu \frac{\partial H_y^f}{\partial t} = \frac{\partial E_z^f}{\partial x} - \frac{\partial E_x^f}{\partial z} \tag{10}$$

TE second harmonic field

$$\varepsilon_y \frac{\partial E_y^s}{\partial t} = \left(\frac{\partial H_x^s}{\partial z} - \frac{\partial H_z^s}{\partial x}\right) - 2\varepsilon_o d_{14}\frac{\partial}{\partial t}\left(E_x^f E_z^f\right) \tag{11}$$

$$\mu \frac{\partial H_x^s}{\partial t} = \frac{\partial E_y^s}{\partial z} \tag{12}$$

$$\mu \frac{\partial H_z^s}{\partial t} = -\frac{\partial E_y^s}{\partial x} \tag{13}$$

3. SOLUTION METHOD AND NUMERICAL RESULTS

The finite-difference time-domain (FDTD) method is used to numerically solve Equations (8) to (13). The method is suitable for this application because of its ability to include different structures and different media. It is also capable of producing results for multiple frequencies using a single

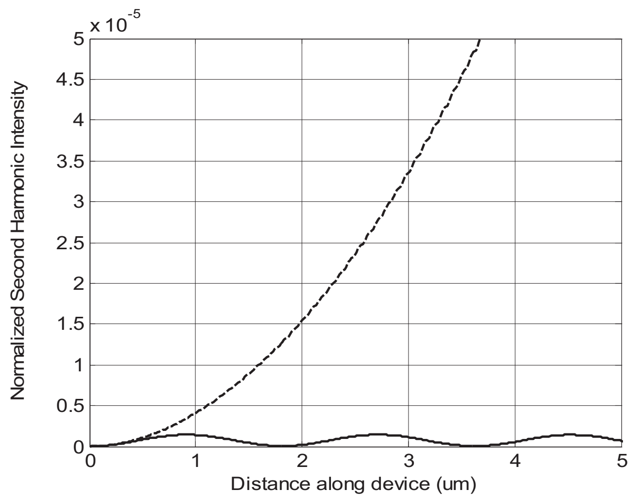

Figure 1: SHG along the nonlinear waveguide (solid: no matching, dashed: perfect match).

simulation. To increase the accuracy of the computations, the PML absorbing boundaries are used for the truncation of the computation domain. A symmetric GaAs-based dielectric slab waveguide is considered to test the proposed FDTD algorithm. It consists of a 0.44-μm thick guiding layer sandwiched between two 3-μm thick AlAs layers. The arrangements of the field components for both the fundamental and second harmonic are made according to the standard Yee cell. The excitation field is a CW TM signal at a fundamental wavelength of $\lambda_f = 1.064\,\mu\text{m}$ and an amplitude of 5.0 A/μm. The transverse profile of the excitation corresponds to the first TM guided mode at the given operating frequency. For the sake of illustration, two matching scenarios are considered. First, no matching technique is used such that the level of coupling between the input and the generated waves depends entirely on the phase shift between them. This phase shift is defined by the difference between the effective indices of the two coexisting guided modes. Second, the effective refractive index of the first odd guided mode of the TE field at $\lambda_s = 0.533\,\mu\text{m}$ is perfectly matched to the first even guided mode of the TM input field by numerically changing the value of the refractive index of the guiding layer at λ_s. The results for both scenarios are shown in Figure 1. As expected, energy exchange between the fundamental field and the second harmonic field takes place periodically during every coherence length if no matching technique is implemented. If, however, the two waves are perfectly matched, the energy exchange will be continuous, resulting in a coherent build-up of the second harmonic energy. The transverse profiles for the fundamental TM mode and the second harmonic TE mode are shown in Figure 2. The simulation verifies the

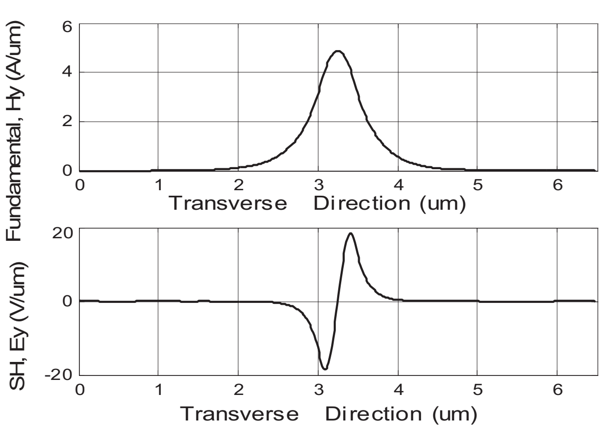

Figure 2: TM input (fundamental) and generated TE second harmonic profiles.

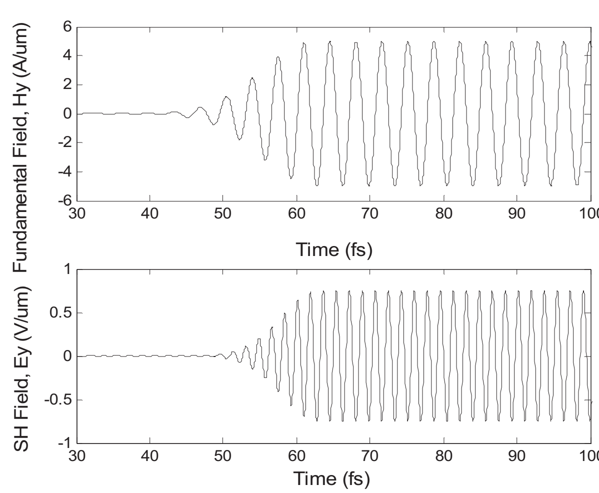

Figure 3: Time-domain results for the fundamental and second harmonic fields at a point along the device at the center of the guiding layer.

coupling of second harmonic energy on the first odd TE mode. Finally, time-domain results of the input fundamental field and the generated second harmonic field at a point along the device are shown in Figure 3. The results confirm the relative frequency between the two propagating beams.

4. CONCLUSIONS

The developed model can be utilized to efficiently analyze and study different optical structures with second order nonlinearities. Instead of calculating the total field inside the structure and then performing spectral analysis to separate the two propagating waves, the presented model solves directly for the fundamental as well as the second harmonic fields. It should find application in a wide range of device structures and in the analysis of short-pulse propagation in second order nonlinear devices. The extension of the model for applications involving pulsed excitations and different device geometries is a future work.

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