Accurate Time Domain Method for Simulation of Microstructured Electromagnetic and Photonic Structures

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Abstract-A time-domain numerical model within the framework of transmission line modeling (TLM) is developed to simulate electromagnetic pulse propagation inside multiple microcavities forming photonic crystal (PhC) structures. The model developed is quite general and is capable of simulating complex electromagnetic problems accurately. The field quantities can be mapped onto a passive electrical circuit equivalent what ensures that TLM is provably stable and conservative at a local level. Furthermore, the circuit representation allows a high level of hybridization of TLM with other techniques and lumped circuit models of components and devices. A photonic crystal structure formed by rods (or blocks) of high-permittivity dieletric material embedded in a low-dielectric background medium is simulated as an example. The model developed gives vital spatio-temporal information about the signal, and also gives spectral information over a wide frequency range in a single run. The model has wide applications in microwave communication systems, optical waveguides and electromagnetic materials simulations.

Keywords—Computational Electromagnetics, Numerical Simulation, Transmission Line Modeling.

I. INTRODUCTION

TRADITIONALLY, the experimental realization and theoretical study of complex electromagnetic systems involving fine features, compound geometries and material properties is technically very difficult and limited to simple design variations. Complex systems, for example photonic crystals (PhCs) consisting of material with periodic variation in the refractive index such as in photonic waveguides [1, 2], can be accurately studied in simulation, and the results obtained can give a useful insight into the physics of these systems before actually building them, which is extremely beneficial for systems where there is substantial complexity in fabrication. Simulation aided research can often lead to more rapid or fully developed results [3]. Particularly, time domain numerical methods such as the Finite Difference Time Domain (FDTD) [4] or the Transmission Line Modeling (TLM) [5] method are specially attractive in electromagnetics for problems involving complex material parameters such as nonlinearity and dispersion, since the EM signal and its spatial and temporal transformations can be tracked accurately, and also the spectral characteristics can be obtained over a wide frequency range in a single run by using Fourier transform in conjunction with these methods.

In this paper a rigorous vectorial TLM model for Gaussian pulse propagation through a two-dimensional PhC consisting of square blocks (cavities) of a high dielectric constant material embedded in a background medium of lower dielectric permittivity material is developed. The model is based on direct discretization of well-known Maxwell's equations that form the basis of electromagnetics [6].

It is worth mentioning here some of the salient features of the TLM algorithm vis-à-vis other standard methods, such as the widely used FDTD method, that has been extensively used for numerical simulation of electromagnetic systems and devices. TLM utilizes the concepts of transmission line theory to model electromagnetic material properties and systems [7, 8]. The problem space is discretized into sections of transmission lines, connected with each other at nodes. These transmission line sections are then represented by a combination of equivalent lumped circuit components whose parameters are chosen so as to represent the properties of the background material. Additional lumped components in the form of stubs are connected at the nodes to represent complex material properties and constitutive relations. The TLM method is similar to FDTD method in that both act by direct discretization of Maxwell's differential equations, however, unlike in FDTD where the electric and magnetic fields are separated in space and time by a half of the cell size and a half of the time step respectively, TLM solves for all the fields at the same point in time and space - this makes TLM highly applicable for simulations of EM wave propagation in complex materials, such as frequency dependent, anisotropic and nonlinear materials. Also, an additional advantage when developing TLM algorithm comes from the fact the field quantities are mapped onto a passive electrical circuit equivalent making it provably stable [5]. Furthermore, the circuit representation allows a high level of hybridization of TLM with other techniques and lumped circuit models of components and devices. Unlike one other commonly used

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method (Beam Propagation Method, BPM) [9], the time domain method TLM has no limitation of a requirement of a gradually varying index in the direction of propagation (and thus can simulate high- as well as low-index contrast structures) or of a slowly varying envelope approximation (and thus can successfully simulate ultrafast signal propagation). All these advantages of TLM make it very attractive for application to simulation of complex electromagnetic structures such as PhCs.

II. FORMULATION

At high frequencies such as microwave and optical frequencies, a sensible description of the electromagnetic pulse propagation through complex materials is provided by Duffing equation that is based on the mechanical Lorentz model of displacement of dipoles [10]. The polarization function of a general Duffing model can be written as:

$$\frac{\partial^2 P(y,t)}{\partial^2 t} + 2\delta \frac{\partial P(y,t)}{\partial t} + \omega_0^2 f(P(y,t)) P(y,t)$$

$$= \varepsilon_0(y) \Delta \chi_e(y) \omega_0^2 E(y,t)$$
(1)

Here, P(y,t) represents the polarization in the y-direction, δ is the damping frequency, ω_0 is the resonant frequency, χ_e represents the susceptibility contrast of the material, and t is the time variable. The term f(P(t) in (1) represents a nonlinear function of the polarization. The Duffing model thus represents in general a nonlinear, frequency dependent model. The equation (1) combines the effect of material dispersion given by the Lorentz model and the nonlinearity of the material. As a special case, the above equation can be used to represent a linear material by making f(P(t))=1. Similarly, the equation can be used to represent a dispersion-free material by modifying it as:

$$f(P(x,t))P(x,t) = \varepsilon_0(x)\Delta\chi_e(x)E(x,t)$$
(2)

In (2) above, the derivatives of the polarization w.r.t. time t have been forced to zero to make it frequency-independent. The equations above have been discretized in the current formulation using a Z-transform technique [6, 10] so that

$$\frac{\partial}{\partial t} \to s \to \frac{2}{\Delta t} \left(\frac{1 - z^{-1}}{1 + z^{-1}} \right)$$
(3)

where s is the Laplace variable, and Δt is the TLM time step. For the isotropic, non-magnetic source free region of the dielectric structure being studied, the Maxwell's equations for a two-dimensional space, for a transverse magnetic (TM) mode propagating in the z-direction reduce to a set of three equations given as:

$$\frac{\partial E_{y}}{\partial x} = -\mu_{0} \frac{\partial H_{z}}{\partial t}$$
(4)

$$\frac{\partial E_{y}}{\partial z} = \mu_{0} \frac{\partial H_{x}}{\partial t}$$
(5)

$$\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} = \varepsilon_0 \frac{\partial E_y}{\partial t} + \frac{\partial P_y}{\partial t}$$
(6)

The polarization equation (1) is then solved along with the standard Maxwell's equations (4)-(6) and the constitutive relations to get the response of the system. Here, in this work, a condensed shunt-node formulation was used to solve the modes corresponding to the TM case. The boundary conditions at the discontinuities in the dielectric material in the direction of propagation as well as in the transverse direction were accounted for in the Maxwell's equations.

III. SIMULATION RESULTS

To demonstrate the application of the TLM model developed to analyze the mcrocavities, a background medium (free space in this case) represented by 400 TLM cells in the longitudinal z-direction and 370 TLM cells in the transverse x-direction is considered, where one TLM cell equals $\Delta z = (-\Delta x) = 1.66 \times 10^{-8}$ m. To begin with, a single cavity of material with refractive index 3.35 and represented by 9x9 TLM cells embedded in the background medium is considered, which will be extended to more complex structures later. A short Gaussian plane wave is launched towards the microcavity, as shown schematically in Fig.1.



Fig. 1 The schematic arrangement showing a Gaussian plane wave launched into a microcavity consisting of 9x9 TLM cells.

The width of the Gaussian envelope is equal to 500 TLM time steps, where one TLM time step equals $\Delta z/\sqrt{2}c$ with *c* as the velocity of light, resulting in temporal width of 19.64 *fs*. The temporal evolution of the signal towards the other side of the cavity is observed with respect to time, and is shown in Fig. 2. Also shown for comparison in the same figure is the temporal evolution when the cavity is not present (i.e. free space). It can be observed that the main peak in the presence of the cavity is followed by ripples that are a result of the energy trapped inside the cavity and being released gradually. The spectrum of the output signal calculated by using FFT technique when the cavity is present is shown in Fig.3, showing the redistribution of the pulse energy due to the presence of cavity.



Fig. 2 The temporal evolution of the Gaussian pulse on the other side of the cavity. Corresponding free space case is also shown for comparison.



Fig. 3 The FFT of the signal in two cases.

This simple case of a single microcavity is now extended to more complex structures by taking the following cases: (i) a single row of such seven cavities in the longitudinal direction, (ii) a single column of such seven cavities in the transverse direction, (iii) and finally an array (7x7) of such cavities, representative of a PhC waveguide, embedded in the free space, and the above measurements are repeated for these special cases, as shown in Fig. 4. Also shown in inset in this figure is the column, row and array of cavities.



Fig. 4 The signal evolution in case of one row of cavities (solid line), one column (line with points) and 7x7 array (dotted line).

It can be observed from Fig. 4 that in case of a row of cavities, the peak of the signal increases beyond the normalized value of unity, followed by an undershoot. This effect is not so prominent in case of a column. This feature is observable in case of the array, and the signal propagation is delayed. This takes place because of the interaction and periodic transfer of the energy trapped in various cavities. A map of the field pattern for the three cases after 1024 TLM steps is shown in Fig.5.



Fig. 5 The map of the field after 1024 time steps for (a) row of cavities, (b) column of cavities, and (c) array of cavities.

IV. CONCLUSION

An accurate time domain numerical method based on the direct discretisation of Maxwell's differential equations has been developed and applied to the simulation of multiple cavities embedded in a background medium, in the form of a 2-D photonic crystal waveguide. The method is quite general and can be extended and applied to more complex structures such as nonlinear cavities resulting in optical switching, a uniform periodic cavity array with missing rows etc. The method is of significance since it gives important information about the spatio-temporal dynamics of the pulse and is not based on any inherent assumptions.

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