Computation of the Filtering Properties of Photonic Crystal Waveguide Discontinuities Using the Mode Matching Method

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Abstract—In this paper, the application of the Mode Matching (MM) method in the case of photonic crystal waveguide discontinuities is presented. The structure under consideration is divided into a number of cells, which supports a number of guided and evanescent modes. These modes can be calculated numerically by an alternative formulation of the plane wave expansion method for each frequency. A matrix equation is then formed relating the modal amplitudes at the beginning and at the end of the structure. The theory is highly efficient and accurate and can be applied to study the transmission sensitivity of photonic crystal devices due to fabrication tolerances. The accuracy of the MM method is compared to the Finite Difference Frequency Domain (FDFD) and the Adjoint Variable Method (AVM) and good agreement is observed.

Keywords—Optical Communications, Integrated Optics, Photonic Crystals, Optical Waveguide Discontinuities.

I. INTRODUCTION

PHOTONIC Crystals (PCs) [1],[2] are constantly attracting increased attention as a potential solution for the realization of ultra-compact integrated optical circuits. The strong confinement of light in a PC waveguide (PCW) allows the design of sharp waveguide bends in which light can change direction 90° without significant power losses [3]. This is in contrast to conventional low index-contrast integrated optical components in which the bending radii must be kept rather large (in order to limit the bending losses). Large bending radii may increase the overall size of the integrated circuit such as the Arrayed Waveguide Grating [4]. PC-based devices can perform much photonic functionality such as light generation [5] and processing [6]. Various designs have also been demonstrated for optical filtering [7]-[11]. Many of the aforementioned designs are based on the introduction of discontinuities (defects) inside a PCW.

Finite Difference Time Domain (FDTD) [12] is an accurate method for studying electromagnetic problems including the simulation of many PC-based devices. The main drawback of this method is that as the device under consideration increases in size the method demands increased memory resources and computational time. Especially in the case of PCW, long Perfectly Matched Layer (PML) sections must be used in the input and output of the device in order to prevent reflections [13]. In addition, the size of the grid can pose restriction in modelling small dimensional fluctuations due to fabrication imperfections. On the other hand the Finite Difference Frequency Domain (FDFD) method [14] could be modified in order to account for small geometry perturbations [15] but requires prohibitively large memory resources in order to solve a practical PC based device problem.

In this paper, we demonstrate the effectiveness of an alternative method based on Mode Matching (MM) [16] in the analysis of PCW discontinuities, such as the ones encountered in PC-based filters. It is shown that the MM method can provide accurate results, even for small variations of the geometrical parameters, without requiring significant memory resources and computational time. In the framework of the MM method, whenever a discontinuity is encountered inside a waveguide, evanescent modes are excited and we attempt to match the guided mode in the PCW with the modal fields in the discontinuity cell. This allows the computation of the reflection and transmission coefficients of each guided waveguide mode. In this way, the MM method provides a useful physical insight to the problem. Furthermore since in most large device designs, distinct cell types of discontinuities are encountered, one needs to calculate the modal fields only once for each type of cell. This can significantly speed up the computation process.

In practice PC-based devices exhibit imperfections due to fabrication tolerances. It is important to be able to study these devices for small variations from the theoretical device parameters. Finite Difference methods need huge memory resources to take into account such small variations. Adjoint Variable Method (AVM) [15] is an accurate method to determine the sensitivity of a function, for example the reflectivity of a device, with respect to any design parameter.

In this paper we show that the MM method is highly accurate even for small variations of the discontinuities in a PCW and its results are compared to AVM.

The rest of the paper is organized as follows: in section II the modal fields of the PCW and the discontinuity cell are computed for both guided and evanescent modes at a given frequency ω . In section III, the MM method is presented in the

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case of PCW discontinuities and in section V, the results of the MM method are compared to some example cases with the FDFD and AVM.

II. CALCULATION OF THE MODES

In order to implement the MM method, one first needs to calculate the guided and evanescent modes supported by each cell of the structure and their propagation constants β . In general, the evanescent modes of a periodic structure may have complex β [1] and hence, their propagation constants may lie on the entire complex plane and not just on the real or imaginary axis as in constant cross-section waveguides. Hence conventional plane wave expansion method, where ω is calculated for each propagation constant β is not suitable since it is much more preferable to be able to determine the values of $\beta = \beta(\omega)$ corresponding to a given frequency ω .

In this section, a method for determining the evanescent and guided mode properties of a periodic structure at a given ω , is outlined based on the formulation of the source-free Maxwell's equations in terms of a generalized Hermitian eigenproblem as in Ref. [17],[18]. This method will be used in order to calculate the modal fields required in order to implement the MM method illustrated in the next section.

Using Bloch's theorem, the modes of a periodic dielectric structure along the z-direction can be written as in Ref. [2]

$$\mathbf{E}(\mathbf{r}) = \mathbf{u}(\mathbf{r})e^{j\beta z} \tag{1}$$

$$\mathbf{H}(\mathbf{r}) = \mathbf{v}(\mathbf{r})e^{j\beta z} \tag{2}$$

where β is the propagation constant of the mode and **u**,**v** are periodic functions along the z direction. Defining $|\beta\rangle$ to be a four component vector comprising of the tangential parts **u**_t and **v**_t of **u** and **v** respectfully, i.e.

$$|\beta\rangle = (\mathbf{u}_t, \mathbf{v}_t)^T = (u_x, u_y, v_x, v_y)^T$$
(3)

one can write Maxwell's equations in the following form [19]

$$\left(\hat{A} + j\frac{\partial}{\partial z}\hat{B}\right)|\beta\rangle = \beta\hat{B}|\beta\rangle \qquad (4)$$

where the operators \hat{A} and \hat{B} are defined by

$$\hat{A} = \begin{pmatrix} \omega \varepsilon - \frac{1}{\omega} \nabla_{t} \times \frac{1}{\mu} \nabla_{t} \times & 0 \\ 0 & \omega \mu - \frac{1}{\omega} \nabla_{t} \times \frac{1}{\varepsilon} \nabla_{t} \times \end{pmatrix} (5)$$

$$\hat{B} = \begin{pmatrix} 0 & -\mathbf{z} \times \\ \mathbf{z} \times & 0 \end{pmatrix} \tag{6}$$

In (5), ε and μ are the dielectric constant and the magnetic permeability of the structure. The eigenvalues of the eigenproblem (4) can be used to determine the propagation constants of both evanescent and guided modes of the structures while the eigenvectors determine their modal fields. In order to solve (5) one can expand the periodic four component vector in terms of plane and standing waves as

$$|\beta\rangle = \sum_{m>0,n>0,l} \mathbf{B}(\mathbf{G}_{mnl}) \sin\left(\frac{G_{mx}x}{2}\right) \sin\left(\frac{G_{ny}y}{2}\right) e^{jG_{lz}z}$$
(7)

where **B**(**G**_{mnl}) are the Fourier coefficients of $|\beta\rangle$ and we have assumed that the periodic cell is rectangular and in this case **G**_{mnl}=[G_{mx},G_{ny},G_{lz}] where G_{mx}=2 $\pi m/b$, G_{ny}=2 $\pi n/d$, G_{lz}=2 $\pi l/a$ and b,d,a are the sizes of the cell along the x,y and z direction respectively.

Note that the fields in (7) vanish at the edges of the cell and hence the structure can be thought as being enclosed by perfectly conducting walls. This situation is reminiscent to the arguments used to obtain the radiation mode spectrum of a simple slab waveguide [20]. In theory b and d must be taken infinite but similarly to the case of the dielectric slab waveguide, as the walls move further and further apart from the waveguide center, the guided modes of the waveguide remain practically the same while more evanescent modes tend to appear having their field primarily outside the "core" of the PCW. This means that for discontinuities near the core these modes will not be significantly excited and hence will not affect the transmission and reflection of the guided modes. Hence in practice b and d are assumed finite and their value must be taken so that the guided modes of the structure decay significantly near the perfectly conducting walls of the cell.

For a 2D PCW where ε does not change with y, the eigenproblem is further simplified in the Transverse Magnetic (TM_y) case, since one needs to consider only one y-directed electric and one x-directed magnetic field tangential components which we will designate as u_y and v_x . In this case the fields do not depend on y and hence the reciprocal lattice vectors \mathbf{G}_{mnl} are such that $\mathbf{G}_{mnl} = \mathbf{G}_m = [G_{mx0}, 0, G_{lz}]$.

Substituting (7) in (4), and after some mathematical manipulation the operator eigenproblem is transformed to a matrix eigenproblem which is written as

$$M\mathbf{V} = \boldsymbol{\beta}\mathbf{V} \tag{8}$$

where the vector

$$\mathbf{V} = \left(V_{1}, ..., V_{N}, U_{1}, ..., U_{N}\right)^{T}$$
(9)

comprises of all the spectral components $V_1,...,V_N$ and $U_1,...,U_N$ of v_x and u_y respectfully (note that a finite number N of spectral components must be assumed for computational purposes). The $(2N)\times(2N)$ square matrix M depends on ω and contains all information of the dielectric constant expanded in Fourier series.



Fig. 1 A structure comprising of discontinuities with arbitrarily positioned dielectric rods between two PCW cells

III. MODE MATCHING METHOD

In this section the equations related to the MM method are derived. Fig. 1 depicts the general situation where a sequence of N cells containing dielectric rods is considered. The field must satisfy the continuity equations, i.e. the tangential fields at the left of a boundary must equal the tangential fields at the right of the boundary. At the *i*th cell the tangential electric and magnetic fields are written as:

$$\mathbf{E}_{t}^{i} = \sum_{m} a_{m}^{(i)} \mathbf{e}_{tm}^{(i)} e^{j\beta_{m}^{(i)}(z-z_{i-1})} + \sum_{m} b_{m}^{(i)} \mathbf{e}_{tm}^{\prime(i)} e^{-j\beta_{m}^{(i)}(z-z_{i})}$$
(10)

where $\mathbf{e}_{tm}^{(i)}$, $a_m^{(i)}$ and $\beta_m^{(i)}$ are the tangential electric Bloch functions, the coefficients and the propagation constants of the m^{th} forward mode of the i^{th} cell respectively, while $\mathbf{e}_{tm}^{\prime(i)}$ and $b_m^{(i)}$ are the tangential electric Bloch functions propagation constants of the m^{th} backward mode of the i^{th} cell respectively and

$$\mathbf{H}_{t}^{i} = \sum_{m} a_{m}^{(i)} \mathbf{h}_{tm}^{(i)} e^{j\beta_{m}^{(i)}(z-z_{i-1})} + \sum_{m} b_{m}^{(i)} \mathbf{h}_{tm}^{\prime(i)} e^{-j\beta_{m}^{(i)}(z-z_{i})}$$
(11)

where $\mathbf{h}_{im}^{(i)}$, and $\mathbf{h}_{im}^{\prime(i)}$ are the tangential magnetic Bloch functions propagation constants of the m^{th} forward mode and the m^{th} backward mode the i^{th} cell respectively.

At each interface between two cells, the tangential fields must be continuous and at the boundary $z=z_i$ [21], this implies:

$$\mathbf{E}_{t}^{i}(\boldsymbol{z}_{i}) = \mathbf{E}_{t}^{i+1}(\boldsymbol{z}_{i})$$
(12)

$$\mathbf{H}_{t}^{i}(z_{i}) = \mathbf{H}_{t}^{i+1}(z_{i})$$
(13)

Taking the integral of the electric field in (12) multiplied by the magnetic Bloch function of the $(i+1)^{th}$ cell, $\mathbf{h}_{tn}^{(i+1)}$, and the integral of the magnetic field in (13) multiplied by the electric Bloch function of the i^{th} cell, $\mathbf{e}_{tn}^{(i)}$ respectively for $1 \le n \le M$ yields a matrix equation relating the mode coefficients in cells *i* and *i*+1:

$$\begin{pmatrix} \mathbf{A}^{i+1} \\ \mathbf{B}^{i+1} \end{pmatrix} = \mathbf{Z}_i \cdot \begin{pmatrix} \mathbf{A}^i \\ \mathbf{B}^i \end{pmatrix}$$
(14)

where vectors $\mathbf{A}^{i} = [a_{1}^{i}, ..., a_{M}^{i}]^{T}$, $\mathbf{B}^{i} = [b_{1}^{i}, ..., b_{M}^{i}]^{T}$ contain the coefficients of the *M* forward and *M* backward modes for i^{th} cell. The matrix Z_{i} is given by

$$Z_i = Y_i^{-1} X_i \tag{15}$$

where the element of the matrices Y_i and X_i are given by

$$\begin{bmatrix} X_i \end{bmatrix}_{nm} = \begin{cases} \left\langle \mathbf{e}_{tm}^{(i)}, \mathbf{h}_{tn}^{(i+1)} \right\rangle e^{j\beta_m^{(i)}a} & 1 \le m, n \le M \\ \left\langle \mathbf{e}_{tm}^{\prime(i)}, \mathbf{h}_{tn}^{(i+1)} \right\rangle & 1 \le m - M, n \le M \\ \left\langle \mathbf{h}_{tm}^{(i)}, \mathbf{e}_{tn}^{(i)} \right\rangle e^{j\beta_m^{(i)}a} & 1 \le m, n - M \le M \\ \left\langle \mathbf{h}_{tm}^{\prime(i)}, \mathbf{e}_{tn}^{(i)} \right\rangle & M + 1 \le m, n \le 2M \end{cases}$$
(16)

And

$$[Y_{i}]_{nm} = \begin{cases} \left\langle \mathbf{e}_{tm}^{(i+1)}, \mathbf{h}_{tm}^{(i+1)} \right\rangle & 1 \le m, n \le M \\ \left\langle \mathbf{e}_{tm}^{\prime(i+1)}, \mathbf{h}_{tm}^{(i+1)} \right\rangle e^{-j\beta_{m}^{(i+1)}a} & 1 \le m-M, n \le M \\ \left\langle \mathbf{h}_{tm}^{(i+1)}, \mathbf{e}_{tn}^{(i)} \right\rangle & 1 \le m, n-M \le M \\ \left\langle \mathbf{h}_{tm}^{\prime(i+1)}, \mathbf{e}_{tn}^{(i)} \right\rangle e^{-j\beta_{m}^{(i+1)}a} & M+1 \le m, n \le 2M \end{cases}$$
(17)

If the structure consists of many cells, the one can relate the modal amplitudes at the input to the modal amplitudes of the output using the following equation:

$$\begin{pmatrix} \mathbf{A}^{\mathbf{N}} \\ \mathbf{B}^{\mathbf{N}} \end{pmatrix} = \mathbf{Z} \cdot \begin{pmatrix} \mathbf{A}^{\mathbf{1}} \\ \mathbf{B}^{\mathbf{1}} \end{pmatrix}$$
(18)

and the matrix Z is given by

$$Z = Z_{N-1} \cdot \dots \cdot Z_1 \tag{19}$$

To examine the transmission and reflection properties of the

structure one can set all the output backward modes equal to zero and assume that only the guided modes are excited at the input. In this case one obtains

$$\mathbf{B}^{1} = -Z_{22}^{-1}Z_{21}\mathbf{A}^{1}$$
(20)

$$\mathbf{A}^{N} = Z_{11}\mathbf{A}^{1} + Z_{12}\mathbf{B}^{1}$$
(21)

where the matrices $M \times M$ submatrices of Z are determined by

$$Z = \begin{bmatrix} Z_{11} & Z_{12} \\ Z_{21} & Z_{22} \end{bmatrix}$$
(22)

To summarize, in order to calculate the transmission and reflection properties of a structure one can divide it into N sections and calculate the matrices Z_i at each boundary. One can then obtain the Z matrix using (19) and calculate the amplitudes of the coefficients of the backward modes at the input using (20). The modal amplitudes of the forward modes at the device output are given by (21). One can therefore estimate the transmission and reflection coefficients of the guided modes through the structure.

Referring to figure 1, note that at the beginning of the device at $z=z_0$, one can assume that the PCW cells extend infinitely from $z=z_0$ to $z=-\infty$, and hence no mode conversion takes place before the first cell (*i*=1). Similarly and since the backward PCW modes at the last cell (*i=N*) equal to zero, no reflection will occur at the end of the structure. Hence no absorber cells are required at the end of the structure unlike the FDFD method.

IV. RESULTS AND DISCUSSION

A. Comparison with FDFD

To compare the results of the MM method with the FDFD method, one defect rod with radius r_d is placed inside a PC waveguide. Fig. 2 depicts the power reflection calculated with the FDFD (dots) and the MM method (solid lines). The radius of the rods of the PCW was taken $r_a=0.12\mu m$, while the lattice constant was $a=0.6\mu m$. The wavelength in free space was taken λ =1.55µm. The dielectric constant of the rods was assumed $\varepsilon_a = 9\varepsilon_0$ and that of the surrounding medium was $\varepsilon_b = \varepsilon_0$. The radius of the defect r_d varied from $0.1r_a$ to $2.0r_a$. For the calculation of the modes the number of plane waves used was 15 for the propagation direction (z-direction) while 19 standing waves were used for the transverse direction (xdirection). The grid of the FDFD was taken $\Delta = r_a/8$ in order to account for the small variations in the size of the defect rods and 10 PML rods were used along the z-direction in both sides, necessary in order to minimize reflections from the edge of the computational window [13]. Note that the FDFD required more than 1GB of RAM in order to solve its system of equations. On the other hand no serious memory

requirements were imposed by the MM method. Both methods required roughly the same amount of time to produce their results with the MM method being slightly faster. As observed by the figure, there is a very good agreement between the two methods and this verifies the accuracy of the MM method. A similar agreement is obtained when the position of the defect rods is changed. Table I, shows the values for the power reflection calculated with both methods assuming a single defect rod (as in Fig. 2) with $r_d=r_a$ whose position changes $\pm r_a$ in either the x or the z direction. Note that the MM method computes practically the same values for R when the rods are displaced $\pm r_a$ along the x-direction and this is not surprising since the structure is symmetric along this direction. The same is true for the z-direction as well.

 TABLE I

 Comparison between the FDFD and MM Method for Various Defect

 Rod Positions

Position	Power Reflection R		
	MM method	FDFD method	
+ra (x-direction)	0,7781	0,7685	
-ra (x-direction)	0,7727	0,7977	
+ra (z-direction)	0,8286	0,8426	
-ra (z-direction)	0,8286	0,8638	



Fig. 2 Comparison of the MM and the FDFD methods for single defect rod inside a PC-waveguide

B. Comparison with AVM

To verify the accuracy of MM method for small geometrical perturbations of a discontinuity in a PCW, we introduce one defect rod with radius $r_d=1.2r_a$ inside the PC waveguide and calculate the power reflectivity of the device by changing the defect radius by $\pm 1\%$ (figure 3). The rest of the PC parameters (lattice constant a, rod radius ra, etc) are the same as in section IV A. The results are compared with the AVM in figure 4. AVM is used to calculate the sensitivity of the power reflectivity of the PCW with one defect rod, with respect to the defect rod radius. To implement this method the Maxwell equations were solved in the frequency domain using the FDFD and the sensitivity is calculated by considering the adjoint problem as outlined in [15]. The grid of the FDFD was taken $\Delta = r_a/6$. As seen in the figure, an excellent agreement is observed in terms of the slope of the variation of the

reflectivity in terms of the defect rod radius. This confirms the applicability of the MM method for the study of small structural deviations in PC-based devices.



Fig. 3 A PCW with one defect rod introduced in the waveguide. The structure is divided in two different types of cells



Fig. 4 Power reflectivity of a PCW with one defect rod introduced in the waveguide. The defect rod radius is altered by 1% and the sensitive of the power reflectivity with respect to the defect radius is calculated with MM and AVM

V. CONCLUSION

The mode matching method has been applied in the study of PC-based waveguide discontinuities. The method is based in the expansion of the field in terms of the eigenmodes of the cells of the structure and their matching at the boundary interfaces. The method was verified by comparing it to FDFD simulations. The method has proven to be accurate even for small geometrical variations of the PC parameters. MM method can provide useful physical insight and can be useful in the designs of PC optical filters based on waveguide discontinuities.

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