Efficient Numerical Method for Analyzing Coupling Structures of Photonic Crystal Waveguides

Zhen Hu and Ya Yan Lu

***Abstract*—Efficient coupling of light into and out of photonic crystal (PhC) waveguides is important for applications in photonic integrated circuits. An efficient numerical method is presented for analyzing two-dimensional structures that connect PhC waveguides with conventional waveguides (or free space). The method relies on rigorous boundary conditions for terminating both types of waveguides to obtain small computation domains. These boundary conditions are derived from square root operators for conventional waveguides and Bloch mode expansions in PhC waveguides.**

***Index Terms*—Optical waveguides, photonic crystals, numerical methods, boundary conditions, Bloch mode expansions, Dirichlet-to-Neumann maps.**

I. Introduction

To realize many applications of photonic crystals (PhCs), it is necessary to have efficient coupling of light between a PhC waveguide and a different structure such as a conventional waveguide, a different PhC waveguide or the free space [1]–[4]. In particular, it is quite difficult to couple light into slow-light PhC waveguides. When a PhC waveguide is terminated physically, it may be necessary to minimize reflections at the end facet. For hetero-structures involving two different bulk PhCs, it is necessary to analyze the junctions between different PhC waveguides. Efficient numerical methods can speed up the design and optimization of various structures connecting PhC waveguides. For this type of problems, the finite difference time domain (FDTD) method is widely used, but it requires a proper truncation of the PhC waveguides (which are periodic in the main propagation direction). The perfectly matched layer (PML) technique is widely used, but it is not effective for terminating periodic structures.

In this Letter, we present an efficient frequency-domain method based on rigorous boundary conditions that terminate PhC or conventional waveguides. Assuming that z is the main propagation direction, we divide the entire structure into three regions: $z < 0$, $0 < z < L$ and $z > L$. The left ($z < 0$) and right ($z > L$) regions are PhC waveguides, or conventional waveguides or homogeneous media, while the middle region ($0 < z < L$) corresponds to coupling structures. The special case for $L = 0$ involves only two regions. The key step is to set up rigorous boundary conditions at $z = L^+$ and $z = 0^-$. This allows us to reduce the computation domain to $0 \le z \le L$ (which is just a line if $L = 0$). The boundary conditions involve operators which are approximated by matrices.

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This research was partially supported by a grant from the Research Grants Council of Hong Kong Special Administrative Region, China (Project No. CityU 101706).

II. Conventional waveguides

We consider two dimensional (2D) problems where the structures are invariant in the y direction and light waves propagate in the xz plane. In that case, the governing equation is

$$\rho \frac{\partial}{\partial z}\left(\frac{1}{\rho}\frac{\partial u}{\partial z}\right) + \rho \frac{\partial}{\partial x}\left(\frac{1}{\rho}\frac{\partial u}{\partial x}\right) + k_0^2 n^2\, u = 0, \qquad (1)$$

where k_0 is the free space wavenumber, $n = n(x,z)$ is the refractive index, $\{u, \rho\} = \{E_y, 1\}$ or $\{u, \rho\} = \{H_y, n^2\}$ for the transverse electric (TE) or transverse magnetic (TM) polarization, respectively.

If a conventional waveguide with a refractive index profile $n_0(x)$ is given in the region $z < 0$, we can define the square root operator $\mathcal{B}_0 = i\sqrt{\rho_0 \partial_x(\rho_0^{-1}\partial_x \cdot) + k_0^2 n_0^2}$ (where ρ_0 follows from n_0) by eigenvalue decomposition. Namely, if $\{\phi, \beta^2\}$ satisfy

$$\left[\rho_0 \frac{\partial}{\partial x}\left(\frac{1}{\rho_0}\frac{\partial}{\partial x}\right) + k_0^2 n_0^2\right]\phi = \beta^2 \phi, \quad -\infty < z < \infty, \quad (2)$$

then $\mathcal{B}_0 \phi = i\beta\phi$. The general solution in the waveguide for $z < 0$ can be written as $u = u^+ + u^-$, where u^+ is a given incident field and u^- is the reflected field. Based on the definition of $\mathcal{L}_0$, we have

$$\partial_z u^+ = \mathcal{B}_0\, u^+, \quad \partial_z u^- = -\mathcal{B}_0\, u^-, \quad z < 0.$$

This gives rise to the boundary condition

$$\partial_z u + \mathcal{B}_0\, u = 2\mathcal{B}_0\, u^+ \quad \text{at} \quad z = 0^-. \qquad (3)$$

Similarly, if a conventional waveguide is given in the region $z > L$ and its refractive index profile is $n_1(x)$, we can define the square root operator $\mathcal{B}_1 = i\sqrt{\rho_1 \partial_x(\rho_1^{-1}\partial_x \cdot) + k_0^2 n_1^2}$. If there are only outgoing waves that propagate towards $z = +\infty$ for $z > L$, then the boundary condition is

$$\partial_z u = \mathcal{B}_1\, u \quad \text{at} \quad z = L^+. \qquad (4)$$

If the transverse variable x is discretized by N points, the operators $\mathcal{B}_0$ and $\mathcal{B}_1$ are approximated by $N \times N$ matrices. For ϕ satisfying Eq. (2), a high order three-point finite difference formula derived in [5] gives

$$a_j \phi_{j-1} + b_j \phi_j + c_j \phi_{j+1} \approx d_j \phi''_{j-1} + e_j \phi''_j + f_j \phi''_{j+1}, \quad (5)$$

where $\phi_j = \phi(x_j^+)$ and $\phi''_j = \partial_x^2 \phi(x_j^+)$, etc. As a result, the differential operator $\rho_0 \partial_x(\rho_0^{-1}\partial_x\ ) + k_0^2 n_0^2$ is approximated by

$D_2^{-1}D_1 + D_0$, where D_0 is the diagonal matrix for elements $k_0^2 n_0^2(x_j^+)$, D_1 is the tridiagonal matrix with jth row consisting of a_j, b_j, c_j, and D_2 is the tridiagonal matrix with jth row consisting of d_j, e_j, f_j. This leads to

$$\mathcal{B}_0 \approx i\sqrt{D_2^{-1}D_1 + D_0}. \quad (6)$$

III. PhC waveguides

In a previous work [6], we derived rigorous boundary conditions for terminating PhC waveguides and applied these conditions to analyze PhC devices such as bends, branches, etc. Assuming that a PhC waveguide is given in the region $z < 0$ and it is periodic in z with a period a, then the boundary condition is

$$\partial_z u = \mathcal{L}_0^- u + (\mathcal{L}_0^+ - \mathcal{L}_0^-)u^+, \quad z = 0^-, \quad (7)$$

where u^+ is a given incident field in the waveguide and $\mathcal{L}_0^\pm$ are two operators. The derivation of (7) relies on Bloch mode expansions in the waveguide and the operator M defined below. For one period of the PhC waveguide given by $z_{j-1} < z < z_j$ where $z_j = ja$ for $j \le 0$, the operator M satisfies

$$M \begin{bmatrix} u_{j-1} \\ u_j \end{bmatrix} = \begin{bmatrix} \partial_z u_{j-1} \\ \partial_z u_j \end{bmatrix},$$

where u_j, $\partial_z u_j$ denote u and $\partial_z u$ evaluated at $z = z_j^-$, etc. We note that M characterizes one period of the PhC waveguide. Matrix approximations of M can be obtained from related operators (matrices) for the regular and defect unit cells of the PhC waveguide [7]. Bloch modes of the PhC waveguide are special solutions of the form $\Phi(x,z)e^{i\beta z}$, where Φ is periodic in z, and they can be calculated from an eigenvalue problem associated with M [8]. After the Bloch modes are obtained, we can split the field in the PhC waveguide as $u = u^+ + u^-$, where $u^\pm$ are as

$$\begin{aligned} u^+ &= \sum c_j \Phi_j(x,z)e^{i\beta_j z}, \\ u^- &= \sum d_j \Psi_j(x,z)e^{-i\beta_j z}. \end{aligned}$$

The Bloch mode expansions for u^+ and u^- are chosen such that u^+ represents either propagating Bloch modes with a positive power flux or evanescent modes that decay as z is increased (and the opposite for u^-). Using the Bloch mode expansions and the operator M, we can easily find the operators $\mathcal{L}_0^\pm$. The details can be found in [6].

Similarly, if the region $z > L$ is also a PhC waveguide, we can find two operators $\mathcal{L}_1^\pm$ and write down the boundary condition. In particular, if there are only outgoing waves for $z > L$, then the boundary condition is simplified to

$$\partial_z u = \mathcal{L}_1^+ u, \quad z = L^+. \quad (8)$$

IV. Solution in the coupling region

With the boundary conditions at $z = 0^-$ and $z = L^+$, we can solve Eq. (1) in the region $0 \le z \le L$ by various numerical methods. If the coupling region contains structures identical or similar to those of the background PhC, we can use the Dirichlet-to-Neumann (DtN) map method developed in [6], [9].

For the special case of $L = 0$, the problem is reduced to the line at $z = 0$. An equation for u at $z = 0$ can be obtained from the continuity of $\rho^{-1}\partial_z u$. For example, if we have a conventional waveguide and a PhC waveguide for $z < 0$ and $z > 0$, respectively, then the equation is

$$\left(\frac{1}{\rho^+}\mathcal{L}_1^+ + \frac{1}{\rho^-}\mathcal{B}_0\right)u = \frac{2}{\rho^-}\mathcal{B}_0 u^+,$$

where $\rho^\pm$ denotes ρ at $z = 0^\pm$, u^+ is the incident field given in the conventional waveguide and it is evaluated at $z = 0^-$. Similarly, if we have a PhC waveguide for $z < 0$ and a conventional waveguide for $z > 0$, then the equation is

$$\left(\frac{1}{\rho^+}\mathcal{B}_1^+ - \frac{1}{\rho^-}\mathcal{L}_0^-\right)u = \frac{1}{\rho^-}(\mathcal{L}_0^+ - \mathcal{L}_0^-)u^+.$$

Here, u^+ is the incident field given in the PhC waveguide (for $z < 0$) and it is evaluated at $z = 0^-$.

V. Numerical examples

To illustrate our method, we consider two examples in this section. In the first example, a semi-infinite PhC waveguide is connected directly with a semi-infinite slab waveguide, as shown in Fig. 1. The parameters are chosen as in [2]. The bulk

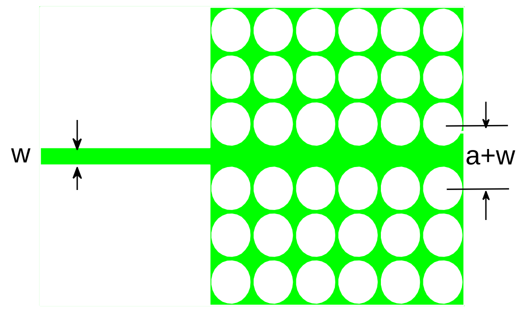

Fig. 1. Direct connection between a PhC waveguide with a slab waveguide.

PhC consists of a square lattice of air-holes in a dielectric medium with refractive index $n = \sqrt{12.96}$. The radius of the air-holes and the width of the slab are $r = 0.45a$ and $w = 0.375a$, respectively, where a is the lattice constant. The PhC waveguide ($z > 0$) is formed by increasing the center-to-center distance between two rows of air-holes to $a + w$. The slab waveguide ($z < 0$) is surrounded by air. The incident field is the fundamental mode of the slab waveguide propagating from left to right (towards the junction). Our objective is to calculate the transmitted power carried by the propagating mode of the PhC, and the reflected power carried by the backward propagating mode of the slab waveguide. For TE polarization and the frequency range $0.22 \le \omega a/(2\pi c) \le 0.245$, both the PhC waveguide and the slab waveguide have only one propagating mode. The transverse variable x is truncated to cover 7 rows of air-holes in each side of the waveguide core, that is, the length of the x interval is $14a + w$. We use 8 collocation points on each edge of the square cells (length a) and 3 collocation points for the core (length w), and obtain a linear system of equations involving only $14 \times 8 + 3 = 115$ unknowns. In Fig. 2, we show the transmitted and reflected powers (normalized by the power of the incident wave), and observe that the power transmission is more than 94% for the frequency range $0.22 \leq \omega a/(2\pi c) \leq 0.245$. Our results are consistent with those reported in [2] where the PhC waveguide is finite.

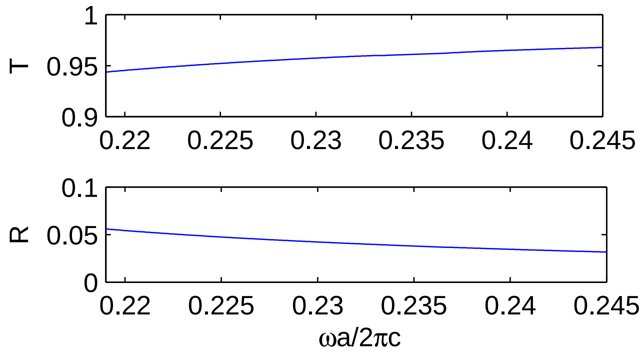

Fig. 2. Transmittance and reflectance of the waveguide junction shown in Fig. 1.

The second example involves a taper between a PhC waveguide given in $z < 0$ and the free space given in $z > L$. The structure was designed by Dossou *et al* [4] to minimize reflections when light propagates out of photonic crystal waveguide. The bulk PhC is a square lattice of circular dielectric rods of radius $r = 0.3a$ and refractive index $n = 3$, where a is the lattice constant. The PhC waveguide is obtained by removing one row of rods along the horizontal z-axis. As shown in Fig. 3, the taper region involves 7 layers ($L = 7a$),

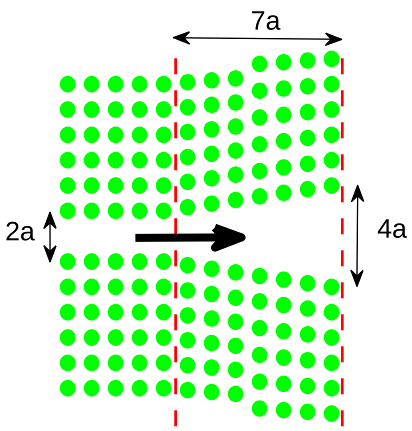

Fig. 3. A PhC waveguide and free space connected by a seven-layer taper.

where the center-to-center distance between the two rods closest to the waveguide core is increased by a factor of

$$w(z) = 2 + 2[(z + 0.5a)/L]^{\xi}, \quad 0 \leq z \leq L. \qquad (9)$$

Our computation domain involves only the seven-layer taper region. Using 5 points on each edge of the unit cells, we obtain a linear system for about 1090 unknowns. The method described in [9] can be used to further speed up the computation. Our results are shown in Fig. 4 and they are indistinguishable to those reported in [4]. Near 100% power transmission is

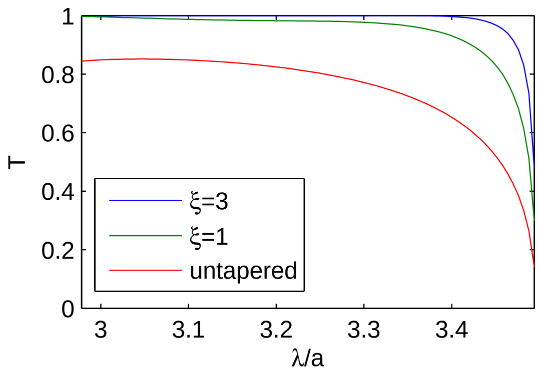

Fig. 4. Transmittance of the tapered and untapered photonic crystal waveguides shown in Fig. 3.

possible for Bloch modes of the PhC waveguide propagating towards free space.

VI. Conclusion

In this Letter, we presented an efficient method to analyze coupling structures for PhC waveguides. We use rigorous boundary conditions to terminate waveguides or homogeneous media, and solve the problem on a reduced computation domain. For PhC waveguides, the boundary conditions are derived from Bloch mode expansions [6]. For conventional waveguides or homogeneous media, we use a high order finite difference scheme to evaluate the boundary conditions involving square root operators. In the reduced computation domain, we can identify unit cells and use DtN maps of the unit cells to avoid their interiors [6]. As a result, the number of unknowns in our method is much smaller than other methods for the same level of accuracy.

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