Novel variational approach for analysis of photonic crystal slabs

Mohammad Hasan Aram and Sina Khorasani
School of Electrical Engineering, Sharif University of Technology, Tehran, Iran
E-mail: khorasani@sina.sharif.edu

Keywords: photonic crystals, slab waveguides, variational methods

Abstract
We propose a new method, based on variational principle, for the analysis of photonic crystal (PC) slabs. Most of the methods used today treat PC slabs as three-dimensional (3D) crystal, and this makes these methods very time and/or memory consuming. In our proposed method, we use the Bloch theorem to expand the field on infinite plane waves, whose amplitudes depend on the component perpendicular to the slab surface. By approximating these amplitudes with appropriate functions, we can find modes of PC slabs almost as fast as we can find modes of two-dimensional crystals. In addition to this advantage, we can also calculate radiation modes with this method, which is not feasible with the 3D plane wave expansion method.

1. Introduction

Ever since the prediction of forbidden gaps in the band structure of some periodic dielectric structures that we now call photonic crystals (PCs) [1], these structures have affected many scientific fields and have found many industrial applications. Today, PCs are used to increase the efficiency of solar cells [2–5], improve lasers and the specs of light-emitting diodes [6–8], and design new kinds of waveguides and optical fibers [9–13]. These nanostructures are a good platform for optical circuits [14, 15] and seem to find applications in new research fields such as quantum information and quantum computation [16–21].

The periodicity of a PC’s dielectric constant can be in one, two, or three dimensions [22–24]. Fabrication of full three-dimensional (3D) PCs or perfect two-dimensional (2D) PCs is difficult and sometimes impossible. This fact has made scientists do their best to work with slabs of PCs because they are fabricated easily with conventional fabrication technologies. PC slabs have periodic permittivity in two dimensions, but finite thickness along the third dimension. They are sometimes known as finite-thickness 2D crystals. These crystals can confine and guide electromagnetic waves according to the distributed Bragg reflection in the plane of the slab and total internal reflection in the slab’s normal direction [11, 25–28]. Up to now, many methods have been proposed for the analysis of PCs. These methods fall into two categories: frequency domain and time domain. Frequency domain methods such as finite element, plane wave expansion, and frequency-difference frequency domains deal with phasors of electromagnetic fields, but time domain methods like the finite-difference time-domain (FDTD) find the fields, evolution according to Maxwell’s equation. Since a PC slab is not a perfect 2D crystal, we need to simulate it as a full 3D crystal, and this has made analyzing it time and/or memory consuming. Some innovative methods have been proposed to solve this problem [29–33], but almost all of them have some shortcomings, including lower accuracy and limited frequency range analysis.

In this paper we introduce our new method, which can find PC slab modes by calculating the eigenvalues of a matrix twice as large as the matrix that appears in the 2D plane wave expansion (PWE) method. Then we obtain the band structure of a sample PC slab and compare it with the results of conventional 3D PWE and FDTD methods. We also compare the eigenfield of this crystal at a high symmetry point obtained from the proposed method with that obtained by the 3D PWE method. To show its ability to analyze PC waveguides, we find guided modes of a sample PC waveguide, and finally we compare the efficiency of this method with the 3D PWE method.
Variational method for PC slab analysis

According to the variational principle, one can find an estimation of the smallest eigenvalues of a Hermitian operator, \( \mathcal{L} \), by choosing a suitable trial function as the eigenfunction of the operator and then trying to minimize

\[
\langle f | \mathcal{L} | f \rangle,
\]

where \( |f\rangle \) is the trial function. In fact, the popular PWE method is based on the variational principle. In this method, the trial function, which is one of the electric or magnetic fields, is chosen according to Bloch theorem to be

\[
\sum \Phi_\kappa(r) \exp(-jG \cdot r),
\]

where \( \Phi_\kappa(r) \) is a periodic function with the same periodicity as that of the dielectric constant of the crystal, \( \kappa \) is the Bloch wave vector, and \( G \) equals \( \sum m_i b_i \), with \( b_i \)'s being the primitive vectors of the reciprocal lattice. The second equality is written by substituting \( \Phi_\kappa(r) \) with its Fourier series expansion. In a PC slab, there is no periodicity in the vertical direction of the slab surface. Hence, to use the standard PWE method, we need to create an artificial periodicity in this direction. This means that we are estimating the field dependency on the normal component of the slab by a Fourier series. Actually this is not a good estimation, because the number of Fourier series coefficients that should be determined can be very large.

Here, we want to show that we can choose a simpler trial function for the field dependency on the normal component of the slab, which results in faster calculation of crystal modes. For clarity of the formulation written in the remainder of the paper, suppose we want to analyze the PC slab shown in Figure 1. This crystal is composed of a triangular lattice of circular air columns etched through a dielectric slab with dielectric constant \( \epsilon_r = 11.9 \) and thickness \( t = 0.6a \), where \( a \) is the lattice constant. The radius of air columns equals \( 0.3a \). According to the Bloch theorem, we can write the magnetic field as

\[
H(r) = e^{-j\kappa \cdot r} \Phi_\kappa(r_{xy}, z),
\]

where \( \Phi_\kappa(r_{xy}, z) \) is a periodic function of \( x \) and \( y \) for every value of \( z \). If we substitute \( \Phi_\kappa(r_{xy}, z) \) by its Fourier series, we can write

\[
H(r) = \sum_G h_G(z) e^{-j(G \cdot r_{x\parallel} + G_z \cdot z)}
\]

where \( e_{G_\parallel} \) and \( e_{G_z} \) are unit vectors along and perpendicular to \( \kappa + G \), respectively. Here, \( G \) is the vector in the reciprocal lattice of a 2D crystal with the same pattern as our PC slab. To find a good estimation for \( h_G(z) \), \( h_{G_\parallel}(z) \), and \( h_{G_z}(z) \), we need to survey the field distribution in a dielectric slab waveguide problem. We know in that problem, amplitudes of guided electric and magnetic fields inside the slab are sinusoidal functions of the \( z \) component, but they decay exponentially outside the slab as \( |z| \) increases--that is,
\[ F_i(r, t) = F_i^{(0)}(z)e^{-\kappa r}e^{i\omega t}, \quad (i = \parallel, \perp, z) \]
\[ = \begin{cases} A_o \sin(kz) \text{ or } A_e \cos(kz), & |z| \leq t/2 \\ C_o e^{-\alpha(z-t/2)}, & z > t/2 \\ C_e e^{\alpha(z+t/2)}, & z < -t/2 \end{cases} \tag{3} \]

where \( F \) stands for electric (\( E \)) or magnetic (\( H \)) fields, \( \omega \) is the angular frequency, and \( A_o, A_e, C_o, C_e, \alpha, \) and \( k \) are constants. It can be shown

\[ \omega^2 = \frac{k^2 + \kappa^2}{\epsilon} \quad \text{and} \quad \alpha^2 = \kappa^2 - \omega^2, \tag{4} \]

where \( \kappa = |\kappa| \). Considering each of the even/odd or transverse-electric (TE)/transverse-magnetic (TM) modes of the waveguide, we can also write four relations between \( \alpha \) and \( k \),

TE: \[ \begin{aligned} \alpha &= k \tan(kt/2) \\ \alpha &= -k \cot(kt/2) \end{aligned} \]

TM: \[ \begin{aligned} \alpha &= k \tan(kt/2)/\epsilon_r \\ \alpha &= -k \cot(kt/2)/\epsilon_r. \end{aligned} \tag{5} \]

We can simply show that the field profiles do not change outside the slab if we carve out the triangular lattice of the circular columns—that is, the electromagnetic field decays exponentially outside the PC slab as \( |z| \) increases. If we can approximate its profile inside the PC slab by sinusoidal functions, then our estimated trial function in a TE-like mode becomes

\[ h_{G_i}(z) = A_{G_i} \begin{cases} \sin(k_{G_i}z), & |z| \leq t/2 \\ \sin(k_{G_i}t/2)e^{-\alpha_{G_i}(z-t/2)}, & z > t/2 \\ -\sin(k_{G_i}t/2)e^{\alpha_{G_i}(z+t/2)}, & z < -t/2 \end{cases} = A_{G_i}f_{G_i}(z) \]

\[ h_{G_x}(z) = A_{G_x} \begin{cases} \sin(k_{G_x}z), & |z| \leq t/2 \\ \sin(k_{G_x}t/2)e^{-\alpha_{G_x}(z-t/2)}, & z > t/2 \\ -\sin(k_{G_x}t/2)e^{\alpha_{G_x}(z+t/2)}, & z < -t/2 \end{cases} = A_{G_x}f_{G_x}(z) \]

\[ h_{G_y}(z) = -j |\kappa + G| A_{G_y} \begin{cases} \cos(k_{G_y}z)/k_{G_y}, & |z| \leq t/2 \\ \sin(k_{G_y}t/2)/\alpha_{G_y}e^{-\alpha_{G_y}(z-t/2)}, & z > t/2 \\ \sin(k_{G_y}t/2)/\alpha_{G_y}e^{\alpha_{G_y}(z+t/2)}, & z < -t/2 \end{cases} = A_{G_y}f_{G_y}(z). \tag{6} \]

\( h_{G_i}(z) \) and \( h_{G_x}(z) \) are chosen to be continuous at \( |z| = t/2 \) and \( h_{G_y}(z) \) is written such that \( \nabla \cdot \mathbf{H}(\mathbf{r}) = 0 \). TM-like mode trial functions can be written in the same manner.

\( A_{G_i}, A_{G_x}, k_{G_i}, k_{G_x}, \) and \( \alpha_{G} \) are parameters that can be determined by minimizing

\[ \frac{\langle \mathbf{H}(\mathbf{r}) | \mathbf{L}_H | \mathbf{H}(\mathbf{r}) \rangle}{\langle \mathbf{H}(\mathbf{r}) | \mathbf{H}(\mathbf{r}) \rangle}, \tag{7} \]

where

\[ \mathbf{L}_H = \nabla \times \left( \frac{1}{\epsilon_0(\mathbf{r})} \nabla \times (\mathbf{H}) \right). \]

This is a time-consuming problem. To further simplify it, suppose we have suitable values for \( \alpha_{G}, k_{G_i}, \) and \( k_{G_x} \).

Then, minimization of expression \( 7 \) becomes minimizing \( \langle A_{G} | \mathbf{M} | A_{G} \rangle \), provided that \( \langle A_{G} | \mathbf{N} | A_{G} \rangle = 1 \),
where

\[
A_G = \begin{bmatrix} A_{G_1} \\ A_{G_2} \end{bmatrix}, \quad \mathcal{M} = \begin{bmatrix} \eta_{G-G} & m_{11} \\ m_{21} & m_{22} \end{bmatrix}_{G,G}
\]

and \( \mathcal{N} = \begin{bmatrix} n_{11} \\ 0 \\ 0 \\ n_{22} \end{bmatrix}_{G,G} \).

In (8), \( \eta_G \) are Fourier series coefficients of \( \eta(r) = 1/\epsilon_r(r) \), and elements of matrices \( \mathcal{M} \) and \( \mathcal{N} \) equal

\[
m_{11} = c_{G_1} \cdot c_{G_2} \left( |\kappa + G|^2 \begin{bmatrix} f'_{G_1}(z) \\ f'_{G_2}(z) \end{bmatrix} + |\kappa + G|^2 \begin{bmatrix} f'_{G_1}(z) \\ f'_{G_2}(z) \end{bmatrix} \right)
\]

\[
m_{12} = c_{G_1} \cdot c_{G_2} \left( \begin{bmatrix} f'_{G_1}(z) \\ f'_{G_2}(z) \end{bmatrix} \right) + |\kappa + G|^2 \begin{bmatrix} f'_{G_1}(z) \\ f'_{G_2}(z) \end{bmatrix},
\]

\[
m_{21} = c_{G_1} \cdot c_{G_2} \left( \begin{bmatrix} f'_{G_1}(z) \\ f'_{G_2}(z) \end{bmatrix} \right) + |\kappa + G|^2 \begin{bmatrix} f'_{G_1}(z) \\ f'_{G_2}(z) \end{bmatrix},
\]

\[
m_{22} = |\kappa + G| \begin{bmatrix} f'_{G_1}(z) \\ f'_{G_2}(z) \end{bmatrix} + e_{G_1} \cdot e_{G_2} \begin{bmatrix} f'_{G_1}(z) \\ f'_{G_2}(z) \end{bmatrix},
\]

\[
n_{11} = \begin{cases} 
\begin{bmatrix} f_{G_1}(z) \\ f_{G_2}(z) \end{bmatrix}, & G = G', \\
0, & G \neq G'.
\end{cases}
\]

\[
n_{22} = \begin{cases} 
\begin{bmatrix} f_{G_1}(z) \\ f_{G_2}(z) \end{bmatrix}, & G = G', \\
0, & G \neq G'.
\end{cases}
\]

Using the Lagrange multipliers method, we can determine \( A_G \) elements by solving the generalized eigenvalue problem,

\[
\mathcal{M} A_G + \lambda \mathcal{N} A_G = 0.
\]

As stated above, we first need to set the values of \( \kappa_G, k_{G_1}, \) and \( k_{G_2} \) to obtain the simplified eigenvalue problem of (10). For this purpose, we temporarily assume angular frequency \( \omega \) to be that of the dielectric slab waveguide, whose same slab thickness and permittivity equals the effective permittivity of PC slab. By effective permittivity, we mean the coefficient of the Fourier series of \( \epsilon_r(r) \) with \( G = 0 \). Please note that we only consider the first band of the dispersion diagram of a slab waveguide—that is, we set

\[
\omega = \omega_1(|\kappa|).
\]

After that, using (4) we can write

\[
\alpha_G = \sqrt{|\kappa + G|^2 - \omega^2},
\]

and then \( k_{G_1} \) and \( k_{G_2} \) are obtained by solving the following equations

**TE-like:**

\[
\begin{align*}
\alpha_G &= k_{G_1} \tan \left( k_{G_1} t/2 \right) \\
\alpha_G &= -k_{G_2} \cot \left( k_{G_1} t/2 \right)/\epsilon_{rt}
\end{align*}
\]

**TM-like:**

\[
\begin{align*}
\alpha_G &= -k_{G_1} \cot \left( k_{G_1} t/2 \right) \\
\alpha_G &= k_{G_2} \tan \left( k_{G_1} t/2 \right)/\epsilon_{rt},
\end{align*}
\]

where \( \epsilon_{rt} \) is the effective permittivity of the PC slab.
3. Results comparison

The calculated TM-like and TE-like band structures of the crystal shown in figure 1 by the proposed variational method have been compared with the results of the standard 3D PWE method in figures 2 and 3. For the PWE method, the number of Fourier series terms in the $xy$ plane was bounded to $N_x = N_y = 5$ and to $N_z = 6$ in the $z$-direction. We also used $N_x = N_y = 5$ for the variational method. One can see that the results have good agreement. In fact, in the TM-like mode, our method gives a more precise result. The discrepancy in high-frequency bands of the TE-like mode is mostly due to the inaccuracy of the 3D PWE method near the light cone. As mentioned, in the 3D PWE method, we need to make an artificial periodicity along the slab’s normal direction by introducing infinite slabs similar to the main slab above and below it. This is done because fields decay exponentially outside the slab, and we can assume that other slabs do not change the field distribution near and inside the main slab. But when we go near the light cone, we are on the edge of the confined and radiation modes of the slab; the field decays slowly outside the slab, and this assumption is not valid any more, so the 3D PWE method loses its accuracy.

One of the advantages of the proposed method over the 3D PWE method is that besides calculating the guided modes of the PC slab, we can also obtain radiation modes by this method. Figure 4 shows guided and radiation TM-like modes of the crystal in figure 1 calculated by the variational method, and compares it with the result of the FDTD method.

**Figure 2.** Comparison of TM-like band structures of the crystal shown in figure 1 obtained by both the variational method and the 3D PWE method. Green region shows the light cone.

**Figure 3.** Comparison of TE-like band structures of the crystal shown in figure 1 obtained by both the variational method and the 3D PWE method.
We have also used our method to plot the TM-like magnetic field distribution in the midplane of the PC slab and in a plane vertical to it at the high-symmetry point of the reciprocal lattice \( M \) (the fifth mode at the \( M \) point), and compared it with the results of the PWE method in figure 5. Again, we see good agreement between the results.

To examine our method’s ability to deal with large unit cell crystals, in figure 6 we plotted a dispersion diagram of a PC slab waveguide by both FDTD and variational methods. This waveguide is built by filling one row of air columns with dielectrics in the \( \Gamma - K \) direction in the crystal of figure 1. This is shown in the upper inset of figure 6, and our method found each of the three guided modes. The lower inset of figure 6 shows the unit cell used to analyze this waveguide. The number of Fourier series terms in the variational method was limited to \( N_x = 7 \) and \( N_y = 23 \), but one can get more accurate results by going beyond these limits.

### 4. Efficiency comparison

It is clear that the proposed method is much faster than the conventional 3D PWE method, because in our method, we have to calculate a matrix whose dimensions are of the order \( O(N^3) \), where \( N \) is the number of Fourier series terms. However, in the 3D PWE method, the matrix dimensions are of the order \( O(N^4) \). To illustrate this fact quantitatively, in figure 7 we have plotted the frequencies of the first TE-like and fourth TM-like modes at high-symmetry points \( M \) and \( K \), respectively, of the crystal in figure 1, versus the time it takes to calculate them. These calculations have been performed with a personal computer equipped with a 32-bit Intel®core™2 Duo CPU. The frequencies are calculated by variational and 3D PWE methods. Results with minimum calculation time are related to \( N_x = N_y = N_z = 1 = 3 \) limitations on terms of the Fourier series, and results with maximum calculation time are related to \( N_x = N_y = N_z = 1 = 8 \). One can see that the variational method converges to the final value at least one order of magnitude faster than the PWE method.

### 5. Conclusions

We presented a new method for fast analysis of PC slabs. In this method, which is similar to the PWE method, instead of creating an artificial periodicity along the normal component of the slab and then approximating the field dependency on this component by a Fourier series, we adopted field distribution in a dielectric slab waveguide to estimate fields in PC slabs. Results of this fast method are in good agreement with those from other standard methods. We also compared the convergence time of our method to the final result with that of the 3D PWE method. Our method shows at least one order of magnitude faster convergence.
Figure 5. TM-like magnetic field distribution at the high-symmetry point \( M(5) \) in the midplane of the crystal from figure 1, obtained from (a) variational and (b) 3D PWE methods. The \( z \) component of the magnetic field in a vertical plane to the crystal obtained from (c) variational and (d) 3D PWE methods.

Figure 6. Dispersion diagram of the PC slab waveguide shown in the upper inset, calculated by both FDTD and variational methods. This waveguide is built by filling one row of air columns in the crystal of figure 1 in the \( \Gamma \rightarrow K \) direction. The lower inset shows the unit cell used for analysis. Magenta regions represent extended modes inside the crystal.
Acknowledgments

This work has been supported by the Research Deputy of Sharif University of Technology, and in part by the Iranian National Science Foundation (INSF) under grant 93026841.

References

[1] Yablonovitch E 1987 Phys. Rev. Lett. 58 2059–62
[2] Zhou D and Biswas R 2008 J. Appl. Phys. 103 093102
[3] Mutitu J G, Shi S, Chen C, Creazzo T, Barnett A, Honsberg C and Prather D W 2008 Opt. Express 16 15238–48
[4] Zeng L, Bermel P, Yi Y, Alamariu B A, Broderick K A, Liu J, Hong C, Duan X, Joannopoulos J and Kimerling L C 2008 Appl. Phys. Lett. 93 221105
[5] Bermel P, Luo C, Zeng L, Kimerling L C and Joannopoulos J D 2007 Opt. Express 15 16986–7000
[6] Hirayama H, Hamano T and Aoyagi Y 1996 Appl. Phys. Lett. 69 791–3
[7] Altug H, Englund D and Vučković J 2006 Nat. Phys. 2 484–8
[8] Ichikawa H and Baba T 2004 Appl. Phys. Lett. 84 457–9
[9] Chutinan A and Noda S 2000 Phys. Rev. Lett. 84 4488–92
[10] Lin S Y, Chow E, Johnson S G and Joannopoulos J D 2000 Phys. Rev. B 62 6212–22
[11] Lončar M, Doll T, Vučković J and Scherer A 2000 J. Lightwave Technol. 18 1402–11
[12] Cerqueira A 2010 Rep. Prog. Phys. 73 024401
[13] McNab S J, Moll N and Vlasov Y A 2003 Opt. Express 11 2927–39
[14] Soljačić M, Luo C, Joannopoulos J D and Fan S 2003 Opt. Express 28 637–9
[15] Akahane Y, Asano T, Song B S and Noda S 2003 Nature 425 944–7
[16] Ohta R, Ota Y, Nomura M, Kumagai N, Ishida S, Iwamoto S and Arakawa Y 2011 Appl. Phys. Lett. 98 173104
[17] Johnson S G, Villeneuve P R and Joannopoulos J D 1999 Science 282 274–8
[18] Brossard F S F, Xu X L, Hadjipanayi M, Hugues M, Hopkinson M, Wang X and Taylor R A 2011 AIP Conf. Proc. 1399 1017–18
[19] Lovtsky A I, Sandris B C and Tittel W 2009 Nature Photon. (London) 3 706–14
[20] Aram M H and Khorasani S 2015 Efficient analysis of photonic crystal slabs J. Laser Opt. Photonics 1 111–22
[21] Shi S, Chen C and Prather D W 2005 Appl. Phys. Lett. 86 1163–5

Figure 7. Convergence time comparison between variational and PWE methods. Frequencies of the first TE-like and fourth TM-like modes at high-symmetry points M and K for the crystal in figure 1 have been plotted versus the time it takes to calculate them. A personal computer equipped with a 32-bit Intel® CoreTM Duo CPU has been used to calculate these frequencies.