Scattering and guidance by photonic crystals consisting of periodic arrays of circular cylinders

Kiyotoshi Yasumoto, Hongting Jia, and Naoya Koike
Department of Computer Science and Communication Engineering
Kyushu University, Fukuoka 812-8581, Japan

ABSTRACT
An accurate semi-analytical approach for modeling electromagnetic scattering and guidance by photonic crystals formed by layered parallel-arrays or crossed-arrays of circular cylinders is presented, using the lattice sums technique, the T-matrix algorithm, and the generalized reflection and transmission matrices for a layered system. The method is quite general and applies to various configurations of photonic crystals consisting a lattice of circular cylinders. The unit cell of array can contain two or more circular cylinders, which may be dielectric, conductor, gyrotropic medium, or their mixture with different sizes. The periodic spacing of cylinders along each array plane should be same over all layers, otherwise the cylinders in different layers may be different in material properties and dimensions.

Keywords: Photonic crystals, scattering, guidance, lattice sums, T-matrix, generalized reflection matrix

1. INTRODUCTION
Photonic crystals are periodic dielectric or metallic structures in which any electromagnetic wave propagation is forbidden within a fairly large frequency range. This frequency range is called the photonic bandgap which is analogous to the electron bandgap in natural crystals. Recently the photonic crystals have received a growing attention, because of their promising applications to the bandgap based optical devices such as narrow-band filters, laser mirrors, high-quality resonant cavities, and photonic crystal waveguides.

A periodic array of infinitely long parallel circular cylinders is typical of discrete periodic systems. The frequency response of the array is characterized by the scattering properties of individual cylinders and the multiple scattering due to the periodic arrangement of scatterers. When the array is layered, it constitutes a photonic crystal. In the layered system, the multiple interaction of space-harmonics scattered from each of array's suppresses the propagation of electromagnetic waves within a particular frequency range and a photonic bandgap is formed. If the layered arrays are embedded in a slab of transparent medium, more variety in the frequency response appears due to the multiple scattering of fields between the array elements and slab boundaries. Although a photonic crystal consisting of layered arrays of parallel cylinders exhibits various interesting features, it is essentially a two-dimensional structure. A fully three-dimensional structure is realized when the axes of parallel cylinders are rotated by a constant angle in each successive layer of the stacking sequence. A photonic crystal waveguide is formed by either surrounding a dielectric space by photonic bandgap materials or introducing a defect into a photonic crystal. The guided fields are strongly confined because any electromagnetic energy can not escape through the surrounding medium.

The electromagnetic scattering and mode guidance by photonic crystals with a lattice of circular cylinders has been extensively investigated, using a method of cylindrical harmonic expansion or computational methods such as the Fourier modal method, the finite element method, the differential method, the finite-difference time-domain technique, and the beam-propagation method. Among those approaches the cylindrical harmonic expansion method is a rigorous analytical one, but it requires a complicated calculation of the periodic Green’s function. Although the computational methods are powerful and can be universally applied to various configurations of photonic crystals, they yield approximate numerical solutions because the electromagnetic boundary conditions between the circular cylinders and the background medium are not rigorously satisfied. A rigorous but concise treatment that takes into account the boundary conditions is an important issue to have better understanding electromagnetic properties of photonic crystals.

In this paper, we shall discuss an accurate semi-analytical approach for analyzing the electromagnetic scattering and guidance by photonic crystals consisting of layered parallel-arrays or crossed-arrays of circular cylinders standing in free space or embedded in a dielectric slab. The approach uses the cylindrical harmonic expansion method combined with the lattice sums technique, the T-matrix algorithm, and the generalized reflection and transmission matrices for a layered system. The reflection and transmission matrices based on the space harmonic fields are first defined for a
periodic array system in isolation. The matrices are expressed in terms of the lattice sums\textsuperscript{14, 15} and the T-matrix\textsuperscript{16} of cylinders located within a unit cell. The lattice sums characterize uniquely a periodic arrangement of scatterers and the details of scattering from each array element are included in the T-matrix, which is obtained in closed form for circular cylinders. The array elements per unit cell can contain two or more cylinders, which may be dielectric, conductor, gyroscopic medium, or their mixtures with different dimensions. When the arrays are layered, the reflection and transmission matrices are concatenated to obtain the generalized reflection and transmission matrices\textsuperscript{17, 18} for the layered system. This yields a recurrence formula\textsuperscript{19} for the generalized reflection and transmission matrices. The dimensions and configurations of cylindrical elements in different layers may be different so long as the array periods are identical over all layers. For an N-layered arrays, the recursion process requires N-l times computations of inversion of matrices. When the layered system consists of identical arrays, a concept of Floquet modes propagating in the layered direction is incorporated\textsuperscript{19} into the concatenation process to calculate the generalized reflection and transmission matrices without using the recursion process.

The generalized reflection and transmission matrices are used to calculate the frequency responses in the reflectance and transmittance of two-dimensional or three-dimensional photonic crystals and to characterize the modal properties of guided waves in two-dimensional photonic crystal waveguides. Various numerical examples are demonstrated to confirm the applicability and accuracy of the method.

2. TWO-DIMENSIONAL SCATTERING

2.1 Reflection and transmission matrices

A periodic array of circular cylinders is free-standing in a background medium with a wave number $k_x$ as shown in Fig. 1. The cylinders are infinite long, parallel to each other, and spaced with a distance $h$ along the x-axis on the plane $y = y_j$, which separates the whole space into two semi-infinite regions assigned $j$ and $j+1$. The local origin of the array is located at $(x_j, y_j)$. We consider the scattering of an electromagnetic plane wave whose direction of incidence is normal to the cylinder axis. The problem is reduced to a two-dimensional one and is treated separately for TM and TE waves relative to the $z$-axis.

Let $k_{o} = k_x \cos \phi_o$ be the x-component of the wave vector of the incident plane wave, where $\phi_o$ denotes the incident angle. The periodic array scatters the incident wave into a series of space harmonics with the wavenumber $k_{nl} = k_x \cos \phi_o + 2\pi l/h$ where $l$ is an integer. The single scattering is characterized by the reflection and transmission coefficients of the array which relate the amplitudes of the reflected and transmitted $l$-th space harmonics to that of the incident plane wave. When the arrays are multilayered as shown in Fig. 2, the scattered space harmonics impinge on the neighbor arrays as new incident waves and are scattered again into another series of space harmonics. This multiple scattering process is described in terms of the reflection and transmission matrices for each of layered arrays, which relate the amplitudes of the reflected and transmitted $l$-th space harmonics to that of the incident $n$-th space harmonic. Taking into account the orthogonality of space harmonic fields, after several manipulations, the reflection matrix $R^j_n (R^j_{-n})$ and the transmission matrix $T^j_n (T^j_{-n})$ for the incidence of space harmonics downgoing (upgoing) toward the $j$-th array are obtained as follows\textsuperscript{5}:

![Figure 1: A periodic array of circular cylinders located on a plane $y = y_j$.](image1.png)

![Figure 2: Layered periodic arrays standing in free space.](image2.png)
\[ R^j_i = X^j_i U^e T_i P^o X^o_i \] (1)
\[ F^o_j = X^o_j (I + U^e T_i P^o) X^o_j \] (2)

with
\[ U^e = \left[ u^e_{i,j} \right] = \frac{2(-i)^m}{k_i h \sin \phi_i} e^{2im\phi_i} \] (3)
\[ X^o_j = \left[ x^o_j \delta_{ij} \right] = [e^{2ik_j \delta_{ij}} \delta_{ij}] \] (4)
\[ \tilde{T}_i = (I - T_i \mathbf{L})^{-1} T_i \] (5)
\[ P^o = \left[ p^o_{i,j} \right] = [u^o m e^{2im\phi_i}] \] (6)
\[ \cos \phi_i \cos \phi_0 + \frac{2\pi}{k_i h}, \quad \sin \phi_i = \sqrt{1 - \cos^2 \phi_i}, \quad \text{Im} \{ \sin \phi_i \} \geq 0 \] (7)

where \( m, n = 0, \pm 1, \pm 2, \ldots \), \( \delta_{ij} \) is the Kronecker’s delta, \( \mathbf{I} \) is the unit matrix, and the array plane \( y = y_j \) is employed as a reference plane for the phase of reflected and transmitted space harmonics. In Eq. (5), \( \tilde{T}_i \) is the T-matrix of the isolated single cylinder located at the local origin \((x_j, y_j)\), \( \tilde{T}_i \) is the T-matrix of the entire periodic array, and \( \mathbf{L} \) is a square matrix whose elements \( L_{mn} \) are given by the \((m-n)\)-th order lattice sums \(14, 15\) as follows:
\[ L_{mn} = S_{m-n}(k_0 h, k_j h \cos \phi_0) = \sum_{l=0}^{\infty} H_l^{(1)}(k_0 h)(k_j h) e^{-jklh \cos \phi_0} (1)^{m-n} e^{jklh \cos \phi_0} \] (8)

where \( H_l^{(1)} \) is the \( n \)-th order Hankel function of the first kind. If both the cylinders and background medium consist of isotropic materials and the cross sections of cylinders are up-down symmetric relative to the array plane \( y = y_j \), we have the following relations:
\[ R^j_i = R^o_j, \quad F^o_j = F^o_j. \] (9)

The lattice sums matrix \( \mathbf{L} \) defined by Eq. (8) characterizes uniquely the periodic arrangement of scatterers and is independent of the polarization of the incident field and the individual configuration of scatterers. The matrix \( \mathbf{L} \) calculated once can be commonly used for both TM and TE waves and for any arrays of cylindrical objects whenever the periods are same. The details of scattering from each array element within a unit cell are described by the T-matrix \( T_i \) in Eq. (5). This is a main advantage of using the lattice sums in the scattering problems for discrete periodic structures. It is well known that the direct sum of Hankel functions in Eq. (8) converges very slowly. To overcome this difficulty, we have derived an integral form \(15\) for the lattice sums which are efficiently calculated using a simple formula of numerical integration for elementary functions.

The T-matrix of cylindrical objects located in a unit cell plays another important role in the present formulation. Any analytical or numerical techniques may be used to calculate the T-matrix. When the cylindrical objects are circular cylinders, in particular, the T-matrix for both two-dimensional TM wave and TE wave excitations is obtained in closed form under various configurations \(19, 22\). For instance, the T-matrix for a circular cylinder of isotropic dielectric of radius \( r_j \), permittivity \( \varepsilon_j \), and permeability \( \mu_j \) located in free space background is given as follows:
\[ T_j = [t_{j,m} \delta_{mn}] \] (10)
\[ t_{j,m} = \frac{e_j / \mu_j \int_{m} (k_0 r_j)^m (k r_j)^m - e_j / \mu_j \int_{m} (k_0 r_j)^m (k r_j)^m}{e_j / \mu_j \int_{m} (k r_j)^m H_m^{(1)}(k_0 r_j) - e_j / \mu_j \int_{m} (k_0 r_j)^m H_m^{(1)}(k r_j)} \quad \text{for TM wave} \] (11)
\[ t_{j,m} = -\frac{\sqrt{\mu_r/\varepsilon_r} J_m(k_n r_j) J'_m(k_n r_j) - \sqrt{\mu_0/\varepsilon_0} J_m(k_n r_j) J'_m(k_n r_j)}{\sqrt{\mu_r/\varepsilon_r} J'_m(k_n r_j) H'_m^{(1)}(k_n r_j) - \sqrt{\mu_0/\varepsilon_0} J'_m(k_n r_j) H'_{m}^{(1)}(k_n r_j)} \quad \text{for TE wave} \] (12)

where \( J_m \) is the Bessel function of the \( m \)-th order. If two or more circular cylinders are contained within a unit cell as shown in Fig. 3, which may be of dielectrics, conductors, gyrotropic materials, or any mixture with different dimensions, the recursive algorithm \(^{16}\) or an aggregate technique\(^{22}\) is used to obtain the T-matrix for the composite cylindrical system in terms of the reduced T-matrix for each cylinder in isolation.

### 2.2 Layered periodic arrays standing in free space

The generalized reflection and transmission matrices of the \( N \)-layered arrays as shown in Fig. 2 can be obtained by successively concatenating the reflection and transmission matrices given by Eqs. (1) and (2). Let \( \tilde{R}_j \) and \( \tilde{F}_j \) be the generalized reflection and transmission matrices for the entire system of \( j \)-layered arrays. When the \((j+1)\)-th array is stacked at \( y = y_{j+1} \) above the \( j \)-th array at \( y = y_j \), \( \tilde{R}_{j+1} \) and \( \tilde{F}_{j+1} \) for this \((j+1)\)-layered system are calculated using the following recursive relations:\(^{18, 19}\)

\[
\tilde{R}_{j+1} = \tilde{R}_j + A_{j+l} \tilde{R}_j Y_j \tilde{F}_j \quad (13)
\]

\[
\tilde{R}_{j+1} = \tilde{R}_j + B_{j+l} \tilde{R}_j Y_j \tilde{F}_j \quad (14)
\]

where

\[
A_{j+1} = F_{j+l} Y_j [I - \tilde{R}_j Y_j \tilde{R}_j Y_j]^{-1} \quad (17)
\]

\[
B_{j+1} = \tilde{F}_j [I - Y_j \tilde{R}_j Y_j \tilde{R}_j]^{-1} Y_j \quad (18)
\]

\[
Y_j = [e^{ik_{j+l}(y_j-y_{j+1})} \sin \phi_j \delta_{m,m'}]. \quad (19)
\]

The generalized reflection and transmission matrices \( \tilde{R}_j^N \) and \( \tilde{F}_j^N \) for the \( N \)-layered arrays are calculated from Eqs. (13)-(16) through the \((N-1)\) times recursion process starting with \( \tilde{R}_0 = R_0 \) and \( \tilde{F}_0 = F_0 \). If the arrays consist of periodically layered identical arrays with an equal separation, \( \tilde{R}_j \) and \( \tilde{F}_j \) are obtained without the recursion process by using the concept of Floquet modes\(^{18}\) in the \( y \) direction. This approach is efficient when the number of arrays is increased. The reflection and transmission efficiencies of the \( N \)-layered arrays into the \( l \)-th space harmonic can be easily calculated from \( \tilde{R}_{N,l}^N \) and \( \tilde{F}_{N,l}^N \) for the incidence of down-going and up-going plane waves, respectively.

### 2.3 Layered periodic arrays embedded in slab

When the array are embedded in a slab of transparent medium as shown in Fig. 4, additional effects are incorporated into the multiple scattering process of the space harmonic fields. These are a change in an effective propagation length of fields inside the slab medium and a multiple scattering of fields between the array planes and the slab boundaries. The combined effects in scattering lend variety to the frequency response of the arrays which may be controllable by varying the slab thickness and material combination. Let the permittivity and permeability of the slab medium be \( \varepsilon_s \) and \( \mu_s \). For an array located in the slab, the reflection and transmission matrices are still given in the form of Eqs. (1) and (2), but the expressions (3), (6), and (7) must be slightly modified due to the Fresnel reflection of space harmonic fields at the plane boundaries between the slab medium and exterior free space as

\[
U^s = [u^s] = \left[ \frac{2(-i)^m}{kh\sin \alpha_i} e^{2\pi i m} \right] \quad (20)
\]

\[
P^s = [p^s_m] = [i^m e^{2\pi i m \alpha_i}] \quad (21)
\]

\[
\cos \alpha_i = \frac{k_s \cos \phi_0 + 2\pi}{kh}, \quad \sin \alpha_i = \sqrt{1 - \cos^2 \alpha_i}, \quad \text{Im} \alpha_i \geq 0. \quad (22)
\]

Since the \( x \) component of the wavevector is conserved through the Fresnel reflection, the lattice sums matrix \( L \) is same as Eq.(8), and hence the array T-matrix \( \tilde{T}_j \) is given by Eq.(7) when \( T \) is replaced by a T-matrix of the cylinder located in the slab medium of infinite extent. For the \( N \)-layered array embedded in the slab, the lower boundary of the slab is treated as the zero-th layer and the upper boundary is as the \((N+1)\)-th layer. Then \( R_{N+1}^N \), \( F_{N+1}^N \), \( R_0^N \), and \( F_0^N \) are replaced
by the conventional Fresnel reflection and transmission matrices which are diagonal matrices. The generalized reflection and transmission matrices \( \tilde{R}^\pm \) and \( \tilde{F}^\pm \) for the embedded \( N \)-layered arrays are obtained\(^9\) from Eqs.(13)-(16) through the \((N+1)\) times recursion process.

2.4 Scattered fields inside layered periodic arrays

The reflected and transmitted fields in the exterior of the layered arrays are easily calculated using the generalized reflection matrix \( \tilde{R}^\pm \) and transmission matrix \( \tilde{F}^\pm \) for the space harmonic fields under the incidence of the plane wave which corresponds to the zero-th space harmonic. However, the calculation of the scattered fields inside the layered arrays requires a different mathematical manipulation due to a nature of the space harmonic expansion of the fields\(^2\). To illustrate the calculation process, we consider a stack of two array elements as shown in Fig. 5. The amplitude of the space harmonics incoming on the \( j \)-th array are denoted by \( a^+_j \) and those of outgoing from the same array are by \( b^-_j \). Then the scattered field within a homogeneous strip region \( y_j < y < y_{j+1} - r_{j+1} \) between two layers of arrays are expressed using a superposition of the space harmonic fields as follows:

\[
\Psi_{j,j+1}(x,y) = g_j(x,y) \cdot b^-_{j+1} + g_j^+(x,y) \cdot b^+_j
\]  

(23)

where

\[
g_j(x,y) = \tilde{g}_j(y-y_j) \cdot e^{ik_j x}
\]  

(24)

\[
v_j(y) = e^{ik_j y}, \quad \kappa_j = k^2 - k'^2.
\]  

(25)

Taking the ray tracing for the space harmonics across the two array elements, on the other hand, we have the following relations:

\[
b^+_{j+1} = \tilde{R}^+_{j+1} \cdot a^-_{j+1}
\]  

(26)

\[
b^-_{j+1} = F^+_{j+1} \cdot a^-_{j+1} + \tilde{F}^+_{j+1} \cdot a^+_{j+1}
\]  

(27)

\[
b^-_{j} = F^-_{j+1} \cdot a^-_{j+1} + \tilde{F}^-_{j+1} \cdot a^+_{j+1}
\]  

(28)

\[
b^+_j = \tilde{R}^-_{j} \cdot V^+(y_{j+1} - y_j) \cdot b^-_{j+1}
\]  

(29)

\[
a_j = V^+(y_{j+1} - y_j) \cdot b^-_{j+1}
\]  

(30)

with

\[
V^+(y) = [v^+_j(y) \delta']
\]  

(31)

where \( \tilde{R}^-_{j+1} \) denotes the generalized reflection matrix of the \((j+1)\)-layered arrays viewed from the down-going incident space harmonics with \( a^-_{j+1} \). Solving Eqs.(26)-(28), \( b^-_{j+1} \) and \( a^+_{j+1} \) are related to \( a^-_{j+1} \) as follows:

\[
b^-_{j+1} = [F^-_{j+1} + \tilde{R}^-_{j+1}(F^+_{j+1})^{-1}(\tilde{R}^+_{j+1} - R^+_{j+1})] \cdot a^-_{j+1}.
\]  

(32)

\[
a^+_{j+1} = (F^+_{j+1})^{-1} \cdot (\tilde{R}^+_{j+1} - R^+_{j+1}) \cdot a^-_{j+1}.
\]  

(33)

From Eqs.(29) and (32), \( b^-_{j+1} \) and \( b^+_j \) appeared in Eq.(23) are related to \( a^-_{j+1} \). Thus the scattered field in the homogeneous strip region \( y_j + r_j < y < y_{j+1} - r_{j+1} \) can be calculated when \( a^-_{j+1} \) is specified. However, this field expression based on the space harmonic expansion does not converge in the inhomogeneous grating region...
which contains the periodic arrays of circular cylinders of radius \( r_{j+l} \). For the grating region, we must turn to the original expression of the scattered field using the cylindrical wave expansion. The incident waves on the \((j+1)\)th array are the down-going and up-going space harmonics with amplitudes \( a_{j+l}^- \). Then the scattered field outside the cylinder within the zero-th unit cell is expressed as follows:

\[
\Psi_{j+l}^-(\rho_0, \theta_0) = [F_j^T \cdot (1 + \mathbf{L} \mathbf{T}_{j+l}) + F_H^T \cdot \mathbf{T}_{j+l}] \cdot (P^+ \cdot a_{j+l}^- + P^- \cdot a_{j+l}^+) \quad (34)
\]

with

\[
F_j = [J_m(k_j \rho_0) e^{i m \theta_0}]
\]

\[
F_H = [H_m(k_h \rho_0) e^{i m \theta_0}]
\]

where \((\rho_0, \theta_0)\) denotes the polar coordinate attached to the zero-th cylinder of the \((j+1)\)th array. Applying the boundary conditions on the cylindrical surface \( r_{j+l} \), from Eq.(34) the scattered field inside the zero-th cylinder are obtained as follows:

\[
\Psi_{j+l}^- (\rho_0, \theta_0) = \mathbf{F}^T_j \cdot \left[ (G_j (1 + \mathbf{L} \mathbf{T}_{j+l}) + G_H \mathbf{T}_{j+l}) \cdot (P^+ \cdot a_{j+l}^- + P^- \cdot a_{j+l}^+) \right]
\]

where

\[
\mathbf{F}^T_j = [J_m(k_j \rho_0) e^{i m \theta_0}]
\]

\[
G_j = \begin{bmatrix} J_m(k_j r_{j+l}) \\ J_m(k_j r_{j+l}) \delta_{m0} \end{bmatrix}
\]

\[
G_H = \begin{bmatrix} H_m(k_h r_{j+l}) \\ J_m(k_h r_{j+l}) \delta_{m0} \end{bmatrix}
\]

Thus the scattered fields \( \Psi_{j+l}^- (\rho_0, \theta_0) \) and \( \Psi_{j+l}^+ (\rho_0, \theta_0) \) within the zero-th unit cell on the \((j+1)\)th layer of array can be calculated using the amplitude \( a_{j+l}^\pm \) of incoming space harmonics, where \( a_{j+l}^- \) is related to \( a_{j+l}^+ \) through Eq.(33). Equations (26)–(33) are recursively used to obtain \( a_{j+l}^\pm \) for all layers of arrays by starting from \( a_{N}^- \) or \( a_{N}^+ \) which is specified by the incident plane wave. This recursion process is performed by a simpler matrix calculus.

3. THREE-DIMENSIONAL SCATTERING

Although the layered array of parallel cylinders exhibits various interesting frequency responses, it is essentially a two-dimensional structure. When the array is illuminated by electromagnetic waves propagating obliquely to the cylinder axis, it is rather difficult to fully control the frequency response by the structural parameters alone. Such a deficiency in the array of parallel cylinders may be improved by introducing a three-dimensional nature in the layering process. The geometry considered here is shown in Fig. 6. Periodic arrays of circular cylinders are stacked in free space with a separation distance \( d_j \) in the \( y \) direction. The cylinders in each layer are infinitely long and parallel to each other, while the cylinder axes are rotated by 90° in each successive layer. The array consisting of \( z \)-directed cylinders is referred to as the \( Z \)-array and the array of \( x \)-directed cylinders is as the \( X \)-array. The cylindrical elements and their periodic spacing may be different in \( Z \)-array and \( X \)-array. The \( z \) components of the incident fields of unit amplitude are expressed as follows:

\[
E_z = E_0 e^{i(k_0 x - k_{0y} y + k_{0z} z)}
\]

\[
H_z = H_0 e^{i(k_0 x - k_{0y} y + k_{0z} z)}
\]

\[
E_z = E_0 e^{i(k_0 x - k_{0y} y + k_{0z} z)}
\]

\[
H_z = H_0 e^{i(k_0 x - k_{0y} y + k_{0z} z)}
\]
\[ E_e = \sin \xi_0 \cos \psi', \quad \mathbf{H}_e = \sin \xi_0 \sin \psi' \]  

(42)

where \( k_{\nu_0} = k_0 \sin \xi_0 \cos \eta_0 \), \( k_{\nu_0} = k_0 \sin \xi_0 \sin \eta_0 \), \( k_{\nu_0} = k_0 \cos \xi_0 \), \( \mathbf{H}_e = \sqrt{\epsilon_0 / \mu_0} H_e' \) is the normalized magnetic field, \( (\xi_0, \eta_0) \) is the angle of incidence and \( \psi' \) is the polarization angle of the incident electric field as depicted in Fig. 6. Since the structure is periodic both in \( x \) and \( z \) directions, the incident field are scattered into a set of space harmonics varying as \( \exp \{ k_{\nu_0}(x + k_{\nu_0} z) \} \) where \( k_{\nu_0} = k_{\nu_0} + 2\pi n / h x \), \( k_{\nu_0} = k_{\nu_0} + 2\pi m / h z \), \( h_x \) and \( h_z \) are the periodic spacing in the Z-array and X-array, respectively, and \( n \) and \( m \) are integers denoting the order of space harmonics. Since the wavevector of the incident plane wave is not perpendicular to the cylinder axis, the scattering by a cylindrical element turns to a three-dimensional problem. The incident TM or TE wave is scattered into both TM and TE waves. In a periodic array, the scattering process between the TM and TE waves takes place sequentially along the array elements. Although such a multiple coupling of scattered fields makes the treatment intricate, being compared with the two-dimensional problem, the approach based on the lattice sums and T-matrix can be also applied to the three-dimensional problem. We formulate the scattering problem by employing \( E_z \) and \( \mathbf{H}_z \) as the leading fields, the scattering problem can be formulated in a similar way as in the two-dimensional problem. Following the analytical procedure the reflection and transmission matrices for the \( Z \)-array and \( X \)-array separately. The results are used to derive the reflection and transmission matrices for the \textit{crossed-array} which doubles the \( Z \)-array and \( X \)-array and constitutes a unit cell in the stacking sequence. The generalization of reflection and transmission matrices for the layered system Fig. 6 are obtained by concatenating those of the \textit{crossed-array} over the repeating number of cell in the \( y \)-direction.

3.1 Z-arrays

The scattering problem is formulated by employing \( E_z \) and \( \mathbf{H}_z \) as the leading fields. The fields can be characterized in terms of the amplitudes \( \{ e_{z, l, m} \} \) and \( \{ \mathbf{H}_{z, l, m} \} \) for each of space harmonics. Let \( e_z \) and \( \mathbf{H}_z \) be the column vectors of \((2L + 1) \times (2M + 1)\) dimensions defined as

\[ e_z = [e_z(-M) L e_z(0) L e_z(M)]^T, \quad e_z(m) = [e_z(-M) L e_z(0) L e_z(M)]^T \]  

(43)

\[ \mathbf{H}_z = [\mathbf{H}_z(-M) L \mathbf{H}_z(0) L \mathbf{H}_z(M)]^T, \quad \mathbf{H}_z(m) = [\mathbf{H}_z(-M) L \mathbf{H}_z(0) L \mathbf{H}_z(M)]^T \]  

(44)

where \( l = \pm L \) and \( m = \pm M \) denote the orders of truncations of space harmonics. Following the analytical procedure \(^{25}\) developed for a problem of three-dimensional scattering from a periodic array of circular cylinders, the amplitude vectors \( \{ e_z^r, \mathbf{H}_z^r \} \) and \( \{ e_z^t, \mathbf{H}_z^t \} \) of the reflected and transmitted waves are related to the incident ones \( \{ e_z^i, \mathbf{H}_z^i \} \) as follows:

\[ \begin{bmatrix} e_z^r \\ \mathbf{H}_z^r \end{bmatrix} = \begin{bmatrix} \mathbf{R}_p & \mathbf{R}_p^{tb} \\ \mathbf{F}_p & \mathbf{F}_p^{tb} \end{bmatrix} \begin{bmatrix} e_z^i \\ \mathbf{H}_z^i \end{bmatrix} \]  

(45)

\[ \begin{bmatrix} e_z^t \\ \mathbf{H}_z^t \end{bmatrix} = \begin{bmatrix} \mathbf{F}_p & \mathbf{F}_p^{tr} \\ \mathbf{R}_p & \mathbf{R}_p^{tr} \end{bmatrix} \begin{bmatrix} e_z^i \\ \mathbf{H}_z^i \end{bmatrix} \]  

(46)

where \( \mathbf{R}_p \) and \( \mathbf{F}_p \) \( (\mathbf{R}_p = e e e h h h h h h) \) of \((2L + 1) \times (2M + 1)\) dimension are the reflection and transmission matrices of the \( Z \)-array. The elements of \( \mathbf{R}_p \) and \( \mathbf{F}_p \) are expressed in terms of the three-dimensional T-matrix \(^{26}\) of the \( z \)-directed cylinder for the incidence of plane wave with the \( z \) dependence of \( \exp \{ \imath k_{\nu_0} z \} \) and the one-dimensional lattice sums calculated as follows:

\[ L_{\nu_0} = S_{\nu_0} (\nu_0 h_z ; k_{\nu_0} \sin \xi_0 \cos \eta_0) \]  

(47)

where \( \nu_0 = \sqrt{k_{\nu_0}^2 - k_{\nu_0}^2} \). Note that \( \mathbf{R}_p^{zh}, \mathbf{R}_p^{zh}, \mathbf{F}_p^{zh}, \) and \( \mathbf{F}_p^{zh} \) represent the cross scattering effects inherent in the three-dimensional scattering.

3.2 X-arrays

Employing the \( E_x \) and \( \mathbf{H}_x \) fields as the leading fields, the scattering problem can be formulated in a similar way as in the \( Z \)-array. The fields are characterized in terms of the amplitudes \( \{ e_{x, m, l} \} \) and \( \{ \mathbf{H}_{x, m, l} \} \) of each of space harmonics. Let \( e_x \) and \( \mathbf{H}_x \) be the column vectors of \((2M + 1) \times (2L + 1)\) dimensions defined as

\[ e_x = [e_x(-M) L e_x(0) L e_x(M)]^T, \quad e_x(1) = [e_{x, -M} L e_{x, 0} L e_{x, M}]^T \]  

(48)

\[ \mathbf{H}_x = [\mathbf{H}_x(-M) L \mathbf{H}_x(0) L \mathbf{H}_x(M)]^T, \quad \mathbf{H}_x(1) = [\mathbf{H}_{x, -M} L \mathbf{H}_{x, 0} L \mathbf{H}_{x, M}]^T \]  

(49)
Then the amplitude vectors \((\mathbf{g}_x^r, \mathbf{h}_x^r)\) and \((\mathbf{g}_x^t, \mathbf{h}_x^t)\) for the reflected and transmitted waves are related to the incident ones \((\mathbf{g}_x^i, \mathbf{h}_x^i)\) as follows:

\[
\begin{bmatrix}
\mathbf{g}_x^r \\
\mathbf{h}_x^r
\end{bmatrix} = \mathbf{R}_x \begin{bmatrix}
\mathbf{g}_x^i \\
\mathbf{h}_x^i
\end{bmatrix} = \begin{bmatrix}
\mathbf{R}^{ee}_x & \mathbf{R}^{eh}_x \\
\mathbf{R}^{he}_x & \mathbf{R}^{hh}_x
\end{bmatrix} \begin{bmatrix}
\mathbf{g}_x^i \\
\mathbf{h}_x^i
\end{bmatrix}
\]

\[
\begin{bmatrix}
\mathbf{g}_x^t \\
\mathbf{h}_x^t
\end{bmatrix} = \mathbf{F}_x \begin{bmatrix}
\mathbf{g}_x^i \\
\mathbf{h}_x^i
\end{bmatrix} = \begin{bmatrix}
\mathbf{F}^{ee}_x & \mathbf{F}^{eh}_x \\
\mathbf{F}^{he}_x & \mathbf{F}^{hh}_x
\end{bmatrix} \begin{bmatrix}
\mathbf{g}_x^i \\
\mathbf{h}_x^i
\end{bmatrix}
\]  

(50)  

(51)

where \(\mathbf{R}^{\mu}_x\) and \(\mathbf{F}^{\mu}_x\) (\(\mu = e, e, h, e, h, h\)) represent the reflection and transmission matrices of the X--array. The elements of \(\mathbf{R}^{\mu}_x\) and \(\mathbf{F}^{\mu}_x\) are expressed in terms of the three-dimensional T-matrix \(S^{x}\) of the x-directed cylinder for the incidence of plane wave with the \(z\) dependence of \(e^{\mu_{k_0x}}\) and the one-dimensional lattice sums calculated as follows:

\[
I_{\text{nr}} = \sum_{m=0}^{\infty} (\zeta^k/m) \sin \zeta_0 \sin m_0
\]  

(52)

where \(\zeta_0 = \sqrt{k_0^2 - k_{0x}^2}\). Note that the order of elements in \(\mathbf{g}_x\) and \(\mathbf{h}_x\) are different from those in \(\mathbf{e}_x\) and \(\mathbf{f}_x\) defined by (43) and (44) for the Z-array.

### 3.3 Crossed-arrays

Assume a crossed-array in which the Z-array and X-array are stacked with a center to center separation of \(d_x\) in the \(y\) direction. The Z-array and X-array in the preceding sections have been treated separately by taking the electric and magnetic fields parallel to the cylinder axis as the leading fields in each configuration. When they are stacked however, the use of common leading fields is requested to describe the multiple scattering process between the two orthogonal arrays in unified manner. Then we choose the \(E_x\) and \(H_x\) fields as the leading fields common to the crossed-array and transform the reflection and transmission matrices of the X-array into those based on \((\mathbf{e}_x, \mathbf{f}_x)\). This calculation is easily performed using the chain matrix which transforms the order of elements of amplitude vector defined by Eqs.(48) and (49) into those of Eqs.(53) and (54) and the linear equations which relate two sets of amplitude vectors \((\mathbf{e}_x, \mathbf{f}_x)\) and \((\mathbf{e}_x, \mathbf{f}_x)\) in the X-array are related to the incident ones \((\mathbf{e}_x, \mathbf{f}_x)\) as follows:

\[
\begin{bmatrix}
\mathbf{e}_x \\
\mathbf{h}_x
\end{bmatrix} = \mathbf{R}_x \begin{bmatrix}
\mathbf{e}_x \\
\mathbf{h}_x
\end{bmatrix} = \begin{bmatrix}
\mathbf{R}^{ee}_x & \mathbf{R}^{eh}_x \\
\mathbf{R}^{he}_x & \mathbf{R}^{hh}_x
\end{bmatrix} \begin{bmatrix}
\mathbf{e}_x \\
\mathbf{h}_x
\end{bmatrix}
\]

\[
\begin{bmatrix}
\mathbf{e}_x \\
\mathbf{h}_x
\end{bmatrix} = \mathbf{F}_x \begin{bmatrix}
\mathbf{e}_x \\
\mathbf{h}_x
\end{bmatrix} = \begin{bmatrix}
\mathbf{F}^{ee}_x & \mathbf{F}^{eh}_x \\
\mathbf{F}^{he}_x & \mathbf{F}^{hh}_x
\end{bmatrix} \begin{bmatrix}
\mathbf{e}_x \\
\mathbf{h}_x
\end{bmatrix}
\]

(53)  

(54)

Now the reflection and transmission matrices \((\mathbf{R}^+_x, \mathbf{F}^+_x)\) and \((\mathbf{R}^-_x, \mathbf{F}^-_x)\) of the Z-array and X-array for the incidence of down-going space harmonics have been obtained as Eqs.(53) and (54) based on the common leading fields \(E_x\) and \(H_x\). When the cylinders are isotropic and up-down symmetric with respect to each array plane, it follows that the reflection and transmission matrices for the incidence of up-going space harmonics are also given by \((\mathbf{R}^+_x, \mathbf{F}^+_x)\) and \((\mathbf{R}^-_x, \mathbf{F}^-_x)\). Then the reflection and transmission matrices for the crossed-array are derived by linking \((\mathbf{R}^+_x, \mathbf{F}^+_x)\) and \((\mathbf{R}^-_x, \mathbf{F}^-_x)\) through the Z-array and X-array stacked with a separation distance \(d_x\). For the incidence of down-going space harmonics from the upper region of the Z-array, after several manipulations\(^{-7}\), the reflection and transmission matrices \(\mathbf{R}^{x+}_x\) and \(\mathbf{F}^{x+}_x\) of the crossed-array are obtained as follows:

\[
\mathbf{R}^{x+}_x = \mathbf{R}^+_x + \mathbf{F}^+_x \mathbf{A} \mathbf{Y} \mathbf{R}^-_x \mathbf{Y} \mathbf{F}^-_x
\]

\[
\mathbf{F}^{x+}_x = \mathbf{F}^+_x \mathbf{A} \mathbf{Y} \mathbf{F}^-_x
\]

(55)  

(56)

with

\[
\mathbf{A}_x = [\mathbf{I} - \mathbf{Y} \mathbf{R}_x \mathbf{Y} \mathbf{R}_x^{-1}]^{-1}
\]

\[
\mathbf{Y}_{x} = [\mathbf{e}^{\delta} \mathbf{F}^{(n)d}_x]^{-1}
\]

(57)  

(58)
where $\kappa(m) = \sqrt{k_0^2 - k_m^2}$. Similarly, the reflection and transmission matrices $R_x^{(1)}$ and $F_x^{(1)}$ for the incidence of up-going space harmonics from the lower region of the $X$-array are obtained as follows:

$$R_x^{(+)} = R_{\perp} + F_{\perp} Y_x R_x Y_x F_{\perp}$$

(59)

$$F_x^{(+)} = F_{\perp} B_x Y_x F_{\perp}$$

(60)

where

$$B_x = [I - Y_x R_{\perp} Y_x R_p]^{-1}.$$  

(61)

3.4 Layered crossed-arrays

Let us consider a 2N-layered arrays in which the $Z$-array and $X$-array are stacked one after the other in the $y$ direction as shown in Fig. 6. This structure may be treated as an $N$-stacking sequence of the crossed-array whose reflection and transmission matrices $R_x^{(1)}$ and $F_x^{(1)}$ are defined by Eqs. (55), (56), (59), and (60). The generalized reflection and transmission matrices for the $N$-layered crossed-arrays are obtained by concatenating $R_x^{(1)}$ and $F_x^{(1)}$ successively over $N$ layers as described in 2.2. Although the notations are a little intricate, the mathematics and analytical procedure are quite straightforward. The generalized reflection and transmission matrices of layered crossed-arrays are calculated by using the three-dimensional T-matrix of an isolated circular cylinder and the lattice sums for one-dimensional periodic array.

4. TWO-DIMENSIONAL PHOTONIC CRYSTAL WAVEGUIDES

The side view of a two-dimensional waveguide is shown in Figure 7. The guiding region $-t < y < t$ is bounded by two photonic crystals. The upper region 1 and the lower region 2 consist of $N_1$-layered and $N_2$-layered arrays of circular cylinders, respectively, which are infinitely long in the $z$ direction and periodically spaced with a common distance $h$ in the $x$ direction. The cylindrical elements should be same along each layer of the arrays but those in difference layers need not be necessarily same in material properties and dimensions. Figure 7 shows a typical configuration in which the identical arrays of circular cylinders with the same radius $r$ and permittivity $\varepsilon$, and permeability $\mu$, are layered with an equal spacing $d_1, d_2$ along the $y$ direction in the upper (lower) region. The parameter $w$ indicates the displacement of the elements along the $x$ direction. The background medium is a homogeneous dielectric with permittivity $\varepsilon_0$ and permeability $\mu_0$. The guided waves are assumed to be uniform in the $z$ direction and vary in the form $e^{i\beta z}$ in the $x$ direction where $\beta$ is a real propagation constant.

The scattering from each layer of the arrays is characterized by the reflection and transmission matrices for the space harmonics with the $x$-dependence as $e^{i\beta x}$ where $\beta = \beta + 2\pi n / h$. For the waveguide shown in Fig. 8, the upper and lower boundaries viewed from the guiding region are characterized by the generalized reflection matrices $R_x^{(1)}$ at $y = t$ and $R_x^{(1)}$ at $y = -t + 0$. Using the analytical procedure described in 2.2, these matrices are calculated as functions of $\beta$. Denoting the amplitude vectors of space harmonics incoming and outgoing for the plane $y = t - 0$ by $a_n^-$ and $b_n^+$, and those for the plane $y = -t + 0$ by $a_n^-$ and $b_n^+$, respectively, the following relations are obtained:

$$b_n^- = R_x^{(1)} a_n^-$$

(62)

$$b_n^+ = R_x^{(1)} a_n^-$$

(63)

$$a_n^+ = \beta \cdot b_n^-$$

(64)

$$a_n^- = \beta \cdot b_n^-$$

(65)

where

$$\beta = [\varepsilon^{(2)\kappa}_{\beta}, \mu^{(2)\kappa}_{\beta}, \delta_{xy}]$$.

(66)

Using Eqs. (62)-(65), the following relation is derived:
Equation (67) has nontrivial solutions only for discrete values $\beta_n$ of $\beta$ which satisfy the dispersion equation

$$\det[\mathbf{I} - \beta \mathbf{R}^u(x)] = 0.$$  

The value of $\beta_n$ gives the propagation constant of the $n$-th guided mode propagating along the $x$ axis. The result is substituted into Eq. (67) to determine the amplitude vectors $a_{n_1}$, $a_{n_2}$, $b_{n_1}$, and $b_{n_2}$ for the $n$-th mode. The mode field distribution in the plane transverse to the $x$ axis can be calculated using a recursion formula starting from $a_{n_1}$ and $a_{n_2}$ as described in 2.4. The mode-field pattern varies within a unit cell along the $x$ axis but the same pattern is repeated with the period $h$.

### 5. NUMERICAL EXAMPLES

Although a substantial number of numerical examples could be generated, we shall discuss here the numerical examples for the reflection properties of the layered parallel arrays embedded in a dielectric slab, the reflection properties of the layered crossed-arrays standing in free space, and the mode guidance in two-parallel photonic crystal waveguides. The numerical results in what follows were obtained by taking account of the lowest seven space harmonics and truncating the cylindrical wave expansion at $m = \pm 10$ to calculate the T-matrix of isolated circular cylinder.

Figure 8 shows the power reflection coefficients $|R_0|^2$ of the fundamental space harmonic ($l = 0$) as functions of the normalized wavelength $h/\lambda_x$ for the normal incidence of (a) TM wave and (b) TE wave into 9-layered arrays of parallel circular cylinders embedded in a dielectric slab. The parameters shown in Fig. 4 are $r = 0.2 h, e_r/e_0 = 1.3, \mu_0/\mu_a = 1.0, d = 9 h, d_1 = d_3 = 0.5 h$, and $d_2 = d_4 = h$. The dotted lines are for dielectric cylinders with $e_r/e_0 = 1.30, e_s/e_0 = e_u/e_0 = e_v/e_0 = 1.2$, and the dashed lines are for air holes with $e_r/e_0 = e_s/e_0 = 1.0$. The solid lines are the dielectric slab without arrays. The dielectric slab is almost completely transparent for the incidence of both TM and TE waves when the cylindrical arrays are not contained. However, there appear several sharp resonance peaks in the reflectance when the arrays are embedded. The number of peaks and the locations of peaks change sensitively depending on the slab thickness, the material constants of cylinders and slab, the
radii of cylinders, and the number of layers and separation
distance of the embedded arrays. Figure 9 shows similar
plots of reflectance for the TM wave normally incident on
9-layered arrays of perfect conductor embedded in a
dielectric slab of thickness $d = 8.2h$, where $d_5 : d_9 = h$,
$d_3 = d_7 = 0.1h$, and other parameters are same as those in
Fig. 8. The dashed line indicates the result for the
dielectric slab without arrays and the dotted line is for the
embedded arrays when all cylinders has a same radius
$r_1 : r_5 = 0.1h$. For the solid line, the radii of cylinders in
succeeding layers are varied such that $r_1 = 0.1h$,
$r_4 = r_6 = 0.86h$, $r_5 = r_9 = 0.054h$, $r_2 = r_8 = 0.24h$, and
$r_3 = r_7 = 0.008h$. It is seen that the embedded arrays of
perfect conductor exhibit a characteristic of a low-pass
filter. There appear several small ripples in the reflectance
of the pass-band when the layered arrays are formed by an
identical array. These ripples can be suppressed by
properly apodizing the radii of cylinders in the succeeding
array elements and very fine characteristics of pass-band
and stop-band are obtained.

Next example is the reflection characteristics of the
crossed arrays of circular cylinders standing in free space
as shown in Fig. 6. We consider the situation where a
crossed array of perfect conducting cylinders is
periodically stacked over a crossed array of dielectric
cylinders. The stacked two crossed-arrays, corresponding
to 4-layered arrays, constitute a unit cell of the stacking
sequence in the $y$ direction. The reflection efficiency of
the crossed-arrays stacked over 32-unit cells is plotted in
is the lattice constant. The number of rows of the lattice in upper and lower regions is assumed. The permittivity of the dielectric substrate is on the plane is required to realize the phase-matching condition (69). The rate of power transfer also depends on is a nonnegative integer. A very accurate calculation of well satisfies such a requirement.

Let the coupling length be with period . Let the coupling length be an integer. Then the phase-matching condition for a field distributions of the lowest even and odd TE modes for three crossed layered-arrays and the modal properties of two-dimensional photonic crystal waveguides can be obtained by transmission matrices for a layered system. It is shown that the reflection and transmission characteristics of parallel or scattered fields combined with the lattice sums technique, the T-matrix algorithm, and the generalized reflection and is a nature of a periodic system, an is a positive integer. Then the phase-matching condition for a waveguides is described in terms of the difference of odd modes extend over five rows of the lattice outside of the guiding region and exhibit an oscillatory behavior as a consequence of confinement due to the Bragg reflection by the periodic lattice. The coupling length of two waveguides is determined by the propagation constants and field profiles in the even and odd modes. Since the mode field pattern changes as a function of , the multilayered crossed-arrays have several stopbands in which both TM and TE wave components are completely reflected. The locations and widths of the stopbands can be controllable by adjusting the radii of the cylindrical elements.

Finally we discuss the results of a modal analysis of two-parallel photonic crystal waveguides. When two identical photonic crystal waveguides are brought in close proximity, they form a directional coupler which can be used for a variety of applications in integrated optics such as power division, switching, and wavelength or polarization selection. The characteristics of coupling are determined by the propagation constants and field distributions of two eigenmodes, an even mode and an odd mode, supported by the two-waveguides system. Their precise analysis is significantly important to design the coupler. The coupled waveguides is schematically shown in Figure 11. Two parallel identical waveguides with a width , formed by photonic crystals with a square lattice of circular air holes on a dielectric substrate, are separated by rows of the lattice where is the lattice constant. The number of rows of the lattice in upper and lower regions is assumed to be . The permittivity of the dielectric substrate is and the radius of air holes is . Figure 12 shows the dispersion curves and field distributions of the lowest even and odd TE modes for three different number of the separating layers. The field distribution is plotted for a wavelength crossing the homogeneous background free-space. The mode field patterns are rather complicated being compared with those of the conventional dielectric waveguides. The fields of both even and odd modes extend over five rows of the lattice outside of the guiding region and exhibit an oscillatory behavior as a consequence of confinement due to the Bragg reflection by the periodic lattice. The coupling length of two waveguides is described in terms of the difference between the propagation constants of the even and odd modes. Since the mode field pattern changes as a function of with period as a nature of a periodic system, an effective power transfer from one waveguide to the other is obtained when the coupling length takes an integral multiple of . Let the coupling length be where is a positive integer. Then the phase-matching condition for a coupler is given by

\[
\beta_{\text{Even}}(\lambda_n) - \beta_{\text{Odd}}(\lambda_n) = \frac{(2M_2 + 1)\pi}{M_1 h} \tag{69}
\]

where is a nonnegative integer. A very accurate calculation of and as functions of the wavelength is required to realize the phase-matching condition (69). The rate of power transfer also depends on the field profiles of the even and odd modes. The transferred power takes a maximum when the sum and difference of field profiles in the even and odd modes coincides with that of the fundamental mode in each of two waveguides in isolation. We can see that the mode field distributions obtained for well satisfies such a requirement.

6. CONCLUSIONS

We have presented a semi-analytical approach to analyze the electromagnetic scattering and guidance by photonic crystals formed by multilayered periodic arrays of circular cylinders. The method uses the cylindrical wave expansion of scattered fields combined with the lattice sums technique, the T-matrix algorithm, and the generalized reflection and transmission matrices for a layered system. It is shown that the reflection and transmission characteristics of parallel or crossed layer-arrays and the modal properties of two-dimensional photonic crystal waveguides can be obtained by
Fig. 1: Dispersion curves and mode field distributions of the lowest even and odd TE modes in the two-parallel photonic crystal waveguides shown in Fig. 12 for three different numbers $M$ of the separating layers. The lattice elements are air holes of a radius $0.475 a$, the permittivity of the dielectric substrate is $\varepsilon = 12.25$, and the waveguide width is $21.5 a$, where $h$ is the lattice constant.
a simpler matrix calculus based on the one-dimensional lattice sums and the T-matrix of a circular cylinder isolated in free space. The method is rigorous since the electromagnetic boundary conditions on the circular cylinders are fully satisfied and can be applied to photonic crystals with a large difference of refractive indices between the lattice and the background medium. If the lattice element contains two or more circular cylinders in unit cell, the T-matrix is replaced by the aggregate T-matrix for the composite cylindrical system. This extension is straightforward.

REFERENCES


