Bi-directional propagation leaky modes in a periodic chain of dielectric circular rods

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Abstract: In this paper, a periodic chain composed of two-dimensional dielectric cylindrical inclusions was studied based on the Fourier series expansion method with perfectly matched layers. Phase and attenuation constants associated with guided modes, forward propagation leaky modes, and backward propagation leaky modes, were conceptually proposed and numerically examined. In particular, the relationships between the backward propagation mode, leaky mode, and propagation constant were explained in the second-order Bragg reflection region. This simple structure was investigated with the goal of realizing an efficient guiding device. Phase and attenuation constant results were compared with the results obtained using the Lattice Sums technique with the T-matrix approach and FDTD method; very good agreement was observed between these methods.

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1. Introduction

During the last few decades, extensive research has focused on studying and developing novel structures based on photonic crystals composed of multilayered arrays of periodically distributed circular rods [1–13]. A photonic crystal with a complete bandgap has been used to localize electromagnetic waves to specific arrays and to guide electromagnetic wave propagation along certain directions at restricted frequencies. After this discovery, photonic crystals have attracted great interest because of their novel scientific and engineering applications in guiding devices for controlling light propagation. Various analytical and numerical methods have been developed to analyze the photonic crystal waveguides produced by removing a row of either air columns or dielectric rods, which results in multimode guiding [1].

Recently, scientific studies have addressed the possibility of efficiently guiding electromagnetic waves along a chain formed by periodically distributed scattering elements (a simple single-layered structure) [2–4]. Coupled-resonator square dielectric chain optical waveguides have been investigated [5] and linear silver nanoparticle chains have been proposed [6]. Simplicity of design and fabrication is considered as the main advantage of this structure. However, to validate good guiding and propagation properties, detailed theoretical physics studies for the phase and attenuation constants associated with the guiding are needed. In this regard, a Fourier series expansion method (FSEM) combined with perfectly matched layers (PML) was proposed here as an efficient method to rigorously study the guiding and leaky modes of periodic chains of circular rods. By introducing PMLs in the transverse direction (in the upper and lower regions of a one-layered guiding structure) a fictitious periodicity was realized and the original waveguide approximated by one period of the periodic waveguide array. The electric and magnetic fields were expanded in a Fourier series and the problem reduced to a set of linear equations for Fourier coefficients.

In this paper, an infinite periodic chain of circular rods was investigated. In particular, the relationships between the backward propagation mode, leaky mode, and propagation constant were explained in the second-order Bragg reflection region, which has not been clearly indicated in previous reports [2, 4]. Based on FSEM, the phase and attenuation constants associated with the guiding were calculated for the forward propagation, backward propagation, and bi-directional propagation leaky modes conceptually proposed and numerically examined. Phase and attenuation constants results were compared with the results obtained using the Lattice Sums technique with the T-matrix approach and FDTD method and very good agreement was observed between these methods. The effectiveness of the proposed formulation was further demonstrated by focusing on the convergence of the propagation constants, and when PMLs were introduced, a very good convergence was obtained under a smaller fictitious period. Although in the present study the circular rods were considered to be pure dielectric (without intrinsic losses), the problem was generalized to a study of a periodic chain composed of plasmonic nano-cylinders having a complex dielectric permittivity.

2. Formulation of the problem

A two-dimensional infinite periodic chain composed of circular rods was periodic along the x-axis and with the lattice constant \( h \) [Fig. 1]. The scatterers were infinitely long in the z-direction and parallel to each other. The circular rods, having radius \( r \), were assumed to be pure dielectrics, with a relative dielectric permittivity \( \varepsilon \). To implement the FSEM, the structure was bounded by PMLs with thickness \( w \) at a distance \( A/2 \) from the global origin. An array with this structure repeats the same configuration with a fictitious period \( A \) along the y-direction, and therefore, the original structure was approximated by the array’s unit cell...
located in $0 \leq y \leq \Lambda$. Assuming the propagation of the transverse electric (TE; $E_z, H_x, H_y$) wave, the calculation procedure for the transverse magnetic (TM; $H_z, E_x, E_y$) wave. The details of the formulation are omitted in this communication due to the space limitations; readers can refer to our previous reports [14, 15].

Fig. 1. Infinite periodic chain of circular rods along x-axis with lattice constant $h$. Radius and dielectric permittivity of rods were $r$ and $\varepsilon$, respectively. To apply FSEM, the periodic structure was bounded by PMLs at a distance $\Lambda/2$ from the global origin.

First, the main idea of the formulation needed to be described. In the case of the TE wave, Maxwell equations were written as follows:

$$
\nu(y) \frac{\partial}{\partial y} E_z = ik_0 \tilde{H}_x, \quad \frac{\partial}{\partial x} E_z = -ik_0 \tilde{H}_y, \\
\frac{\partial}{\partial x} \tilde{H}_y - \nu(y) \frac{\partial}{\partial y} \tilde{H}_x = -ik_0 \varepsilon(y) E_z
$$

(1)

Where $\tilde{H}_{x(y)} = \sqrt{\mu_0/\varepsilon_0} H_{x(y)}$, $\nu(y) = [1+i\sigma(y)]^{-1}$ denoted the stretched coordinate variable [14] characterizing the assumed PMLs, where $\sigma(y) = \sigma_{max} (1-y/w)^{10}$ was the conductivity function. Under the fictitious periodicity of the system, the electric and magnetic fields were approximated by a truncated Fourier series

$$
E_z = \sum_{m=-M}^{M} e_{z,m}(x) e^{ik_m y}, \quad \tilde{H}_{x(y)} = \sum_{m=-M}^{M} \tilde{h}_{x(y)m}(x) e^{ik_m y}
$$

(2)

Where $k_m = 2m\pi/\Lambda$. Substituting Eq. (2) into (1) and using the orthogonality of the Fourier bases, a set of linear equations for the Fourier coefficients $\{e_{z,m}(x)\}$ and $\{\tilde{h}_{x,m}(x)\}$ were derived as

$$
\frac{\partial^2}{\partial x^2} e_z(x) = -k_0^2 C \cdot e_z(x), \quad \tilde{h}_y(x) = i \frac{1}{k_0} \frac{\partial}{\partial x} e_z(x)
$$

(3)

with

$$
e_z(x) = [e_{z,-M} \ldots e_{z,M}]^T, \quad \tilde{h}_y(x) = [\tilde{h}_{y,-M} \ldots \tilde{h}_{y,M}]^T
$$

(4)

$$
C = N - (VA)^T, \quad [N]_{max} = \frac{1}{\Lambda} \int_0^\Lambda \varepsilon(y) e^{-i(k_0y-x_0)y} dy
$$

(5)
\[ V_{m\nu} = \frac{1}{\Lambda} \int_0^\Lambda v(y)e^{-i(k_0-k_m)y} dy, \quad [A]_{m\nu} = \frac{k_m}{k_0}\delta_{m\nu} \]  
(6)

where \( \delta_{m\nu} \) is Kronecker’s delta, \( k_0 \) the wavenumber in a free space, and \( \epsilon(y) \) the dielectric permittivity along the \( y \)-axis within the period \( 0 \leq y \leq \Lambda \). The eigenvalue \( \xi_n (n=1,2,\cdots,2M+1) \) of matrix \( C \) and the eigenvectors \( P_n \) determined the propagation constant as well as the field distributions for the guided and radiation modes in the assumed waveguide. The solutions to (3) were expressed as

\[
\begin{bmatrix} e_x(x) \\ h_y(x) \end{bmatrix} = FU(x-x') \cdot a(x')
\]
(7)

\[
F = \begin{bmatrix} P & P^- \\ -PB & PB \end{bmatrix}, \quad U(x) = \begin{bmatrix} U^+(x) & 0 \\ 0 & U^-(x) \end{bmatrix}
\]
(8)

with

\[
P = [p_{1,1}, \cdots, p_{1,M}, p_{M+1,1}, \cdots, p_{M+1,M}], \quad U^+(x) = [e^{i\xi_n x} \delta_{n\nu}],
\]
\[
B = [\tau_n \delta_{n\nu}],
\]

\[
a(x) = [a_+(x) \quad a^-(x)]', \quad a_+(x) = [a_{1,1}(x) \quad a_{2,1}(x) \cdots a_{M+1,1}(x) \quad a_{M+2,1}(x)]
\]
(9)

\[
F = \begin{bmatrix} P & P^- \\ -PB & PB \end{bmatrix}, \quad U(x) = \begin{bmatrix} U^+(x) & 0 \\ 0 & U^-(x) \end{bmatrix}
\]
(10)

Where \( a_\nu^\pm(x) \) denoted the amplitudes of the forward and backward propagating \( n \)-th modes. Notably, for TM modes with field components \( (H_z, E_x, E_y) \), Li’s factorization rule [16] should be applied.

Next, each circular rod was divided into an enough number of thin parallel rectangular rods and the unit cell of the periodic chain in the \( x \)-direction replaced by a cascade connection of layered parallel planar waveguides. In each waveguide section, the solutions to (1)–(3) are given by (7)–(9). The boundary conditions for \( E_z \) and \( H_y \) at each step-discontinuity were fulfilled by equating the Fourier coefficients on both sides of the section. The scattering amplitudes over the unit cell along the \( x \)-axis were related through the transfer matrix \( K \) [15]

\[
\begin{bmatrix} a_+^+(h) \\ a_-^+(h) \end{bmatrix} = K \begin{bmatrix} a_+^+(0) \\ a_-^+(0) \end{bmatrix}
\]
(11)

The propagation constant \( \gamma_k = \beta_k + i\alpha_k \) of the \( k \)-th mode was determined as

\[
\gamma_k = -i \log \xi_k / h
\]
(12)

Where \( \xi_k \) is the \( k \)-th eigenvalue of the transfer matrix \( K \).

3. Numerical Results and Discussions

Although a substantial number amount of data was generated, the lowest TE and TH modes in the periodic chain were analyzed at \( r = 0.4167h \) and \( \varepsilon = 2.25 \) [Fig. 1]. The fictitious period \( A \) was equal to \( A = 60h \), the truncation number \( M = 150 \), and the thickness \( w, \sigma_{\text{max}} \), and \( R \) of the PML chosen to be \( h, 8.0, \) and \( 2.1 \), respectively, to efficiently absorb the field and to minimize the influence of PML material loss in the calculation of the attenuation constant [17]. This structure was then considered with the goal of developing an efficient guiding device.
The phase constant $\beta h/\pi$ and attenuation constant $\alpha h/\pi$, as a function of the normalized periodicity $0.1 < h/\lambda_0 < 0.8$ for the TE and TM modes, are illustrated in Figs. 2 and 3 by blue and red lines, respectively. The attenuation constant $\alpha h/\pi$ was very small (on the order of $10^{-9}$) in the normalized periodicity range of $0.1 < h/\lambda_0 < 0.4$ for TE modes and the range of $0.1 < h/\lambda_0 < 0.44$ for TM modes. The attenuation constant results showed the same characteristics with and without PML [Figs. 2(a) and 3(a), and Figs. 2(b) and 3(b), respectively]. Thus, the structure was considered an efficient guiding device in this periodicity range despite the configuration simplicity in which modes were called forward guided modes, with near-field distributions at a typical periodicity $h/\lambda_0 = 0.3$ for finite periodic chain in case of TE mode [Fig. 4(a)]. However, the attenuation constant became very large, on the order of $10^{-2}$, and the phase constant almost equal to 1 and 2 in the range $0.4 \leq h/\lambda_0 < 0.45$ and $0.75 \leq h/\lambda_0 < 0.82$ for TE modes and in the range of $0.44 \leq h/\lambda_0 < 0.47$, and $0.79 \leq h/\lambda_0 < 0.84$ for TM modes due to the stop-band nature characterizing the first and second order Bragg reflection in the periodic structure. In the range $0.45 \leq h/\lambda_0 < 0.75$ for TE modes and $0.47 \leq h/\lambda_0 < 0.79$ for TM modes, the attenuation constant was around the order of $10^{-3}$. In this periodicity range, it was noticed that the propagation constants entered the second-order Bragg reflection region. This was explained as a backward propagating leaky mode that had a negative group velocity with leakage losses. The near field distributions at a typical periodicity $h/\lambda_0 = 0.5$ for finite periodic chain in case of TE mode are shown in Fig. 4(b). Because in this region the phase constant was also expressed as $\beta h/\pi - 2 < 0$ ($\alpha h/\pi > 0$) the direction of the mode propagation was opposite to the normal guided modes ($\beta h/\pi > 0$).

Fig. 2. Phase constant $\beta h/\pi$ and attenuation constant $\alpha h/\pi$ of the TE mode as a function of the normalized periodicity $h/\lambda_0$ at $r = 0.4167h$ and $\varepsilon = 2.25$, $\lambda_0$ is a wavelength in a free space.
In the higher periodicity range $h/\lambda_0 \geq 0.82$ for TE modes and $h/\lambda_0 \geq 0.84$ for TM modes, the attenuation constant returned to the order of $10^{-3}$, because the propagation constants entered the third-order Bragg reflection region. This was explained as a forward propagating leaky mode that had a positive group velocity with leakage losses in opposite to the propagation direction of the second-order Bragg reflection region. In addition, in some narrow range, such as $0.71 \leq h/\lambda_0 \leq 0.73$ for TE modes and $0.51 \leq h/\lambda_0 \leq 0.56$ for TM modes, the attenuation constant was around the order of $10^{-6}$ to $10^{-4}$, with the leakage losses becoming very weak, which was called here as backward guided modes in the second-order Bragg reflection region.

Unlike the structure with PML, it was noticed that without PML, the attenuation constant had both positive and negative values. This was because the waves were not absorbed by the surrounding PML and impinged on neighboring layers [Fig. 5]. Hence, multiple interactions between the adjusted periodic chains makes the attenuation constant either positive or negative.

To validate the accuracy of the FSEM, the results for the phase constant $\beta h / \pi$ and attenuation constant $\alpha h / \pi$ of the TM mode as a function of the normalized periodicity $h/\lambda_0$. Other parameters are the same as those in Fig. 2.
guaranteed the convergence only in case of a real propagation constant \( \alpha h / \pi = 0 \). The phase constant \( \beta h / \pi \) was easily calculated using the LST by solving the following dispersion equation:

\[
\det[I - T(\lambda_0) L(\lambda_0, \beta)] = 0
\]

(13)

where \( L \) is a lattice sum related to the periodic arrangements of the scatterers [18] and \( T \) the T-matrix of the circular rod per unit cell. The polarization property of the mode field was included only in the T-matrix of the circular rod. And we also calculate them by FDTD. A comparison is demonstrated in Table 1.

| \( h/\lambda_0 \) | \( \beta h/\pi \) | \( \alpha h/\pi \) | \( \beta h/\pi \) | \( \alpha h/\pi \) | \( \beta h/\pi \) | \( \alpha h/\pi \) | \( \beta h/\pi \) | \( \alpha h/\pi \) | \( \beta h/\pi \) | \( \alpha h/\pi \) |
|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|
| 0.2100           | 0.4526           | 0.8d-009         | 0.453            | 0.4525           | 8.7d-04          | 0.4306           | 2.8d-7           | 0.4310           | 0.4308           | 4.3d-04          |
| 0.2500           | 0.5505           | 2.7d-009         | 0.551            | 0.5509           | 6.9d-04          | 0.5179           | 8.1d-8           | 0.5180           | 0.5180           | 3.5d-05          |
| 0.3500           | 0.8138           | 1.1d-008         | 0.814            | 0.8148           | 7.3d-04          | 0.7486           | 1.3d-8           | 0.7506           | 0.7498           | 2.2d-04          |
| 0.5500           | 1.3405           | 4.8d-003         | 1.340            | 1.3407           | 5.4d-03          | 1.2593           | 5.4d-4           | 1.2590           | 1.2634           | 3.1d-04          |
| 0.6500           | 1.6297           | 2.0d-3           | 1.630            | 1.6298           | 1.7d-03          | 1.5393           | 5.6d-3           | 1.5385           | 1.5466           | 1.1d-02          |
| 0.7000           | 1.7815           | 9.0d-004         | 1.782            | 1.7857           | 1.2d-03          | 1.6804           | 9.6d-3           | 1.6800           | 1.6850           | 0.5d-02          |

which includes different values of the normalized periodicity \( h/\lambda_0 \) for both TM and TE modes. Very good agreement between these two methods was observed.

\[
\text{Fig. 5. Infinite periodic one-layer chain became a multilayered chain structure if there were no PMLs at the boundaries.}
\]

Finally, the convergence behavior results for with and without PML with \( M = 2.5A/h \) were compared [Figs. 6–8]. When PMLs were implemented, very good convergence of the numerical solutions was achieved for a small value of the fictitious period.
4. Conclusion

A periodic chain composed of two-dimensional dielectric cylindrical inclusions was studied based on the Fourier series expansion method with perfectly matched layers. The phase and attenuation constants associated with the guided modes, forward propagation leaky modes, and backward propagation leaky modes, were conceptually appealed and numerically investigated. The backward propagating leaky mode, which had a negative group velocity, was clearly explained using phase constants. The results for the phase constant were
compared with the Lattice Sums technique combined with the T-matrix approach and very good agreement was observed between these two methods.

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