Symmetrical perturbation analysis of complex two-dimensional photonic crystals

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We study complex photonic crystals with unit cells that include different dielectric cylinders. A symmetrical perturbation approach is developed here which predicts how the band spectrum of the complex structures evolves from the most symmetrical prophase. As a specific example, we apply this symmetrical approach to the analysis of square lattices with alternating layers of dielectric cylinders perpendicular to one selected diagonal of the prophase unit cell. The results are shown to be in agreement with the plane wave calculations of the band spectrum.

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I. INTRODUCTION

In the last few years, the study of periodic dielectric structures has received considerable interest because it provides the ability to prevent the propagation of electromagnetic waves in certain frequency ranges. This results from the removal of degeneracies of the free-photon states at the Bragg planes invoked by the periodicity, which produces so-called photonic band gaps. The existence of gaps, which prohibits the propagation of electromagnetic waves in any direction, provides an opportunity to confine and control the propagation of electromagnetic waves. This isolar property of the photonic crystals can have implications for quantum optics, high-efficiency lasers, and optoelectronic devices. Another application of the photonic crystals follows from their photonic band gaps. The existence of gaps, which prohibits the propagation of electromagnetic waves in any direction, provides an opportunity to confine and control the propagation of electromagnetic waves. This isolar property of the photonic crystals can have implications for quantum optics, high-efficiency lasers, and optoelectronic devices.

Despite the progress that has been made in the application and fabrication of photonic crystals, the search for microstructures that can produce a predictable and tunable band spectrum remains an important issue. A precise knowledge of the band structure is needed to interpret and predict any phenomenon related to either isolating or conducting properties of the photonic crystals. The creation of the gap depends on many factors in the microstructures such as the topology, dielectric contrast ratio, lattice structure, and filling factor. The crucial point in understanding the band spectrum is the symmetry of the lattice. A detailed group-theoretical analysis of the band spectrum of the photonic crystal, giving insight on generation of the photonic band gap, was developed in Refs. 2, 8 and 7. As for controlling the band spectrum, different ways have already been suggested. For example, the reduction of the total symmetry of the crystal can remove some band degeneracies, allowing for the appearance of complete gaps. A widening of the photonic band gap was also previously achieved by inserting a material at well-chosen places in the unit cell. An approach, consisting of a rotation of a two-dimensional periodic system of hard inclusions hosted in air to obtain a tunable phononic band gap width, was suggested in Ref. 13. Cassagne et al. in Refs. 14 and 15 developed a symmetrical model to analyze complex hexagonal photonic-band gap structures based on the idea of representing the complex lattice as two embedded sublattices.

In this paper we present a different symmetrical approach for studying complex two dimensional photonic crystals with a basis consisting of different dielectric cylinders. In contrast to the previous studies, our model systematically follows the generation of the photonic crystal band spectrum coming from the most symmetrical prophase, and is therefore able to predict the opening the band gaps as complexity is introduced into the prophase lattice. As a model material, we consider a square lattice with alternating layers of the dielectric rods perpendicular to a select diagonal of the square. We start from a simple square lattice with one rod in the basis, and then simulate complex lattices by changing the parameters of the rods in layers perpendicular to the main diagonal. However, our model is quite general. It may be easily extended to any many-layer square or hexagonal lattice, and also to other complex lattices, including hexagonal comb-like lattice considered in Refs. 14 and 15.

The outline of this paper is as follows. Our symmetrical model is described in Sec. II. We present the theoretical results for a square lattice with two and three alternating layers in Secs. II A and II B, respectively. We also discuss the case of the many-layer square lattice. In Sec. III we compare our theoretical predictions with the plane wave calculations of the photonic crystals in question. A conclusion is given in Sec. IV.

II. SYMMETRICAL MODEL

In an inhomogeneous dielectric material, Maxwell’s equations can be reduced to the following relation for the electric field $\mathbf{E}$ (Ref. 1)

$$\frac{1}{\epsilon(r)} \nabla \times \nabla \times \mathbf{E} = \frac{\omega^2}{c^2} \mathbf{E}.$$  

(1)

We study the two-dimensional photonic crystals, by assuming that the specimen is uniform along one spatial direction, which we denote by the z axis. In this case the propagation of the electromagnetic waves can be considered only in the x-y
plane, and two polarizations of the electromagnetic field are possible. The first is $E$ polarization, in which $E(\mathbf{r})$ is parallel to the $z$ axis and the magnetic field $H(\mathbf{r})$ is in the $x$-$y$ plane. The second is $H$ polarization, in which $H(\mathbf{r})$ is parallel to the $z$ axis and $E(\mathbf{r})$ is in the $x$-$y$ plane.

The dielectric constant for the periodical system is a position dependent and periodic function of the vector $\mathbf{r}$ in the $x$-$y$ plane, satisfying the relation $\epsilon(\mathbf{r}+\mathbf{R})=\epsilon(\mathbf{r})$, where for any integers $l_{1,2}$, $\mathbf{R}_l=l_1\mathbf{a}_1+l_2\mathbf{a}_2$ defines a two-dimensional Bravais lattice with the unit cell constructed on the primitive translation vectors $\mathbf{a}_1$ and $\mathbf{a}_2$. The magnitude $S=|\mathbf{a}_1 \times \mathbf{a}_2|$ gives the area $S$ of a primitive unit cell of this lattice. For each periodical lattice, the reciprocal lattice can be defined by the translation vectors $\mathbf{G}_n=n_1\mathbf{b}_1+n_2\mathbf{b}_2$, where $n_{1,2}$ are integers, and $\mathbf{b}_{1,2}$ are the primitive translation vectors of the reciprocal lattice determined by $\mathbf{a}_1 \cdot \mathbf{b}_j=2\pi \delta_{ij}$ ($i,j=1,2$). The Wigner-Seitz cell constructed on the $\mathbf{b}_{1,2}$ vectors defines the Brillouin zone for this lattice.

In the framework of the plane wave method, we seek the solution of Eq. (1) as an expansion

$$E(\mathbf{r})=\sum_{j=1}^{3} \sum_{\mathbf{G}} \epsilon_j A^j(\mathbf{k},\mathbf{G}) e^{i(k+\mathbf{G}) \cdot \mathbf{r}},$$

where $\mathbf{k}$ is the two-dimensional reciprocal vector lying inside the Brillouin zone, and $\epsilon_j$ are the Cartesian unit vectors. In this case the problem is reduced to the eigenvalue problem

$$\det \left( \mathcal{H} - \frac{\omega^2}{c^2} \right) = 0,$$

where

$$\mathcal{H}(\mathbf{G},\mathbf{G}') = |\mathbf{k}+\mathbf{G}||\mathbf{k}+\mathbf{G}'| \eta(\mathbf{G}-\mathbf{G}')$$

for the $E$ polarization and

$$\mathcal{H}(\mathbf{G},\mathbf{G}') = (\mathbf{k}+\mathbf{G}) \cdot (\mathbf{k}+\mathbf{G}') \eta(\mathbf{G}-\mathbf{G}')$$

for the $H$ polarization. Here $\eta(\mathbf{G}-\mathbf{G}')$ can be found by a direct Fourier transformation of the function $\epsilon(\mathbf{r})^{-1}$ (inverse expansion method) or by the Fourier transformation of the function $\epsilon(\mathbf{r})$ followed by inverting the resultant matrix $\epsilon(\mathbf{G}-\mathbf{G}')$ (Ho’s method). Both formulations are identical in an infinite-dimensional system. In our theoretical analysis, we determine the $\eta(\mathbf{G})$ as Fourier transforms of the inverse dielectric constant $\epsilon(\mathbf{r})$,

$$\eta(\mathbf{G}) = \frac{1}{S} \int_{\text{unit cell}} \frac{1}{\epsilon(\mathbf{r})} e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r},$$

where the integral is taken over the unit cell.

A. Square lattice with two alternating layers

We start from the square lattice, in which, perpendicular to the selected square diagonal, there are two alternating layers occupied by different rods. This lattice is presented in Fig. 1(a). It is a face centered square lattice with a basis including two different rods. The unit cell is defined by the vectors $\mathbf{a}_1=a(1,1)$ and $\mathbf{a}_2=a(-1,1)$, shown in Fig. 1(a) by solid lines. The point group symmetry of this lattice is $C_{4v}$, which contains all the elements of the simple square lattice. We note that this lattice can be represented as two embedded simple square lattices, determined by the same set of primitive vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, but which are shifted with respect to each other by the vector $\tau=a(1,0)$. These sublattices are shown in Fig. 1(a) by dash-dotted lines. Thus the dielectric constant of such a lattice can be expressed as

$$\frac{1}{\epsilon(\mathbf{r})} = \sum_{\mathbf{G}} \left[ \eta^1(\mathbf{G}) e^{i\mathbf{G} \cdot \mathbf{r}} + \eta^2(\mathbf{G}) e^{i\mathbf{G} \cdot (\mathbf{r}+\tau)} \right].$$

Here $\mathbf{G}=n_1\mathbf{b}_1+n_2\mathbf{b}_2$ ($n_{1,2}$ are integers) are the vectors of the corresponding reciprocal lattice, determined by the primitive vectors $\mathbf{b}_1=\pi/a(1,1)$ and $\mathbf{b}_2=\pi/a(-1,1)$; $\eta^1(\mathbf{G})$ are the Fourier transforms of the inverse dielectric constants [Eq. (6)] for the two selected sublattices. The Brillouin zone of this lattice is well known to be a square. It is shown by the solid lines in Fig. 1(b).

Taking into account that $\mathbf{G} \cdot \mathbf{r}=\pi(n_1 n_2)$, we can express the inverse dielectric constant as a sum of the two potentials
\[
\frac{1}{\varepsilon(r)} = V_0(r) + V_1(r).
\] 

The potential \(V_0\) is written as
\[
V_0(r) = \sum_{G_0} \left[ \eta^1(G_0) + \eta^2(G_0) \right] e^{iG_0 \cdot r}.
\]  

Here the sum is running over the reciprocal vectors of the simple square lattice \(G_0 = (2\pi/a)(n_1, n_2)\), with the direct unit cell determined by the primitive vectors \(a_1^0 = a(1,0)\) and \(a_2^0 = a(0,1)\). This simple square lattice may be obtained from the face centered lattice to be studied in the case of all cylinders being identical.

The potential \(V_1\) has the form
\[
V_1(r) = \sum_{G_0} \left[ \eta^1(G_0 + Q) - \eta^2(G_0 + Q) \right] e^{i(G_0 + Q) \cdot r}.
\]  

Here the summing is over the reciprocal vectors \(G_0\) again, the new reciprocal vector \(Q = (\pi/a)(1,1)\) being selected. We note that the potential \(V_0\) has a periodicity of the simple square lattice, since
\[
V_0(r + R_0) = V_0(r),
\]  

where \(R_0 = l_1 a_1^0 + l_2 a_2^0\). Particularly, \(V_0(r + \tau) = V_0(r)\). We will consider the \(V_0\) potential as a potential of the prophase, characterized by the symmetry of the simple square lattice. The unit cell and Brillouin zone of this lattice are shown by dashed lines in Figs. 1(a) and 1(b), respectively. The area of the unit cell of the face centered lattice is greater than twice the area of the unit cell of simple square lattice of the prophase. The area of the Brillouin zone of the face centered lattice is less than half of the area of the Brillouin zone of the simple square prophase.

The potential \(V_1(r)\) satisfies the relation
\[
V_1(r + R_0) = e^{iQ \cdot R_0} V_1(r)
\]  

and, particularly, \(V_1(r + \tau) = -V_1(r)\). It can be treated as a perturbation which is characterized by the difference in properties of the dielectric rods in the alternating layers. Inclusion of the \(V_1\) potential results in a doubling of the period of the direct lattice and in a complete nesting of the Brillouin zone of the simple square prophase into the Brillouin zone of the perturbative phase. This is governed by the vector \(Q\) shown in Fig. 1(b). We note that points \(\Gamma\) and \(M\) of the prophase will be combined by the vector \(Q\) into one \(\Gamma'\) point of the perturbed phase. All points \(X\) of the prophase are separated by the vector \(Q\). They become the points \(M'\) in the perturbed phase.

The periodicity of the \(V_0\) potential implies that it can mix only the states differing by the reciprocal vectors \(G_0\) of the simple square lattice, while the translation properties of the \(V_1\) potential results in a mixing of the simple square states separated by the vector \(Q\). In order to show this we use the plane wave basis (2), which can be divided into two parts:

\[
E(r) = \sum_{j=1}^{3} \sum_{G_0} \left[ A_{G_0}^1 e^{i(k + G_0) \cdot r} + A_{G_0}^2 e^{i(k + Q + G_0) \cdot r} \right].
\]  

In the case of the \(E\) polarization, only the \(z\) component of the electric field exists and we can drop the \(j\) index. After inserting this expression into Eq. (3), we obtain

\[
(V_0(r) + V_1(r)) \sum_{G_0} \left[ |k + G_0|^2 A_{G_0}^1 e^{i(k + G_0) \cdot r} + |k + Q + G_0|^2 A_{G_0}^2 e^{i(k + Q + G_0) \cdot r} \right]
\]  

\[
= \frac{\omega^2}{c^2} \sum_{G_0} \left[ A_{G_0}^1 e^{i(k + G_0) \cdot r} + A_{G_0}^2 e^{i(k + Q + G_0) \cdot r} \right].
\]  

By multiplying this equation at first by the factor \(e^{-i(k + G_0') \cdot r}\) and then by the factor \(e^{-i(k + G_0' + Q) \cdot r}\) and integrating over the unit cell of the prophase, we arrive at the system

\[
\sum_{G_0} \left[ A_{G_0}^1 |k + G_0'|^2 \eta_{G_0' - G_0} + A_{G_0}^2 |k + Q + G_0'|^2 \eta_{G_0' - G_0 - Q} \right]
\]  

\[
= \frac{\omega^2}{c^2} \left( A_{G_0}^1 + \sum_{G_0} A_{G_0}^2 \Delta_{G_0' - G_0} \right),
\]  

\[
\sum_{G_0} \left[ A_{G_0}^1 |k + G_0'|^2 \eta_{G_0' - G_0 - Q} + A_{G_0}^2 |k + Q + G_0'|^2 \eta_{G_0' - G_0} \right]
\]  

\[
= \frac{\omega^2}{c^2} \left( A_{G_0}^2 + \sum_{G_0} A_{G_0}^1 \Delta_{G_0' - G_0} \right).
\]  

Here

\[
\Delta_{G} = \frac{4}{\pi^2 (2l + 1)(2m + 1)}
\]  

if \(G = 2\pi/a(l,m); \) \(\eta_{G} = \eta^1(G) \pm \eta^2(G) + \delta_{G+Q}^{+}\), where \(\delta_{G+Q}^+\) are the known functions of the \(\eta^1\) of \(\eta^1(G) \pm \eta^2(G) \pm \eta^2(G + Q).\) In the first approximation, we can keep only the term with \(l = m = 0\) in the summations on the right side of Eq. (15), then \(\Delta_{G-4/\pi^2} = \delta_{G,0}\) (the Kronecker’s symbol), while \(\delta_{G} \sim 4/\pi^2(\eta_{G}^1 \pm \eta_{G}^2).\)

By the standard procedure of the replacements \(B_{G}^1 = |k + G|^1 A_{G}^1\) and \(B_{G}^2 = |k + G + Q|^1 A_{G}^2\), we obtain the eigenvalue problem for the symmetric matrix

\[
\sum_{G_0} \vec{\eta}(G_0, G_0) B_{G_0}^2 = \frac{\omega^2}{c^2} B_{G_0}^1
\]  

where
$$\mathcal{H}_{G_0, G'_0} = \begin{cases} |\mathbf{k} + G_0||\mathbf{k} + G'_0| \eta_{G'_0-G_0}^+ & |\mathbf{k} + G_0||\mathbf{k} + \mathbf{q} + G'_0| \eta_{G'_0-G_0}^- - G_0 - \mathbf{q} \\ |\mathbf{k} + G'_0||\mathbf{k} + \mathbf{q} + G_0| \eta_{G'_0-G_0}^- & |\mathbf{k} + \mathbf{q} + G_0||\mathbf{k} + G_0| \eta_{G'_0-G_0}^+ \end{cases}$$

(17)

and

$$\mathbf{B}_{G_0} = \begin{pmatrix} B_{G_0}^1 \\ B_{G_0}^2 \end{pmatrix}.$$  

(18)

In Eq. (17) the matrix elements $\eta_{G'}^+$ are the Fourier transforms of the $V_0$ potential, while $\eta_{G'}$ are the Fourier transforms of the $V_1$ potential.

In the case of the $H$ polarization just the same matrix equation (16) can be obtained but with replacement of the product of the absolute values of the vectors (k + $G_0$) for their scalar product. As follows from Eqs. (16)–(18), the potential $V_1\sim[\eta^1(G_1) - \eta^2(G_1)]$ results in interaction between the plane wave states separated by the wave vector $\mathbf{q}$. If these states have close values of the energy in the prophase then they will dramatically split in the perturbated phase. Therefore, at these points of the Brillouin zone, the band gaps can be expected to be opened.

**B. Square lattice with three alternating layers**

As the next step we consider a square lattice, in which perpendicular to the selected diagonal there are three different alternating layers. This lattice is presented in Fig. 2(a). The unit cell may be selected as a parallelepiped with a basis that includes three different cylinders. The primitive vectors are $\mathbf{a}_1=\alpha(1,-1)$ and $\mathbf{a}_2=\alpha(2,1)$, shown by solid lines in Fig. 2(a). The $C_2$ point group symmetry of this lattice is very low; it includes only the mirror axis (11). We note that this lattice can be represented as three embedded lattices, defined by the same primitive vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, and each successive lattice shifted from the previous lattice by the vector $\mathbf{t}=\alpha(1,0)$. These sublattices are shown by dash-dotted lines in Fig. 2(a). Thus the inverse dielectric constant of such a lattice can be expressed as

$$\frac{1}{\varepsilon(r)} = \sum_{G} [\eta^1(G)e^{iG\cdot t} + \eta^2(G)e^{iG\cdot(t+\tau)} + \eta^3(G)e^{iG\cdot(t+2\tau)}].$$

(19)

Here $G=n_1\mathbf{b}_1 + n_2\mathbf{b}_2$ ($n_{1,2}$ are integers) are the vectors of the corresponding reciprocal lattice, with the primitive vectors $\mathbf{b}_1=(2\pi/3\alpha)(1,-2)$ and $\mathbf{b}_2=(2\pi/3\alpha)(1,1)$; $\eta^{1,2,3}(G)$ are the Fourier transforms of the inverse dielectric constants for the three selected sublattices. The Brillouin zone of this lattice is a pseudohexagon shown by solid lines in Fig. 2(b).

Now we note that $G\cdot \tau = 2\pi(n_1 + n_2)/3$. So the inverse dielectric constant can be expressed as a sum of three potentials

$$V_0 = V_0(r) + V_1(r) + V_2(r).$$

(20)

Here the sum runs over the reciprocal vectors of the simple square lattice $G_0=(2\pi/\alpha)(n_1, n_2)$.

In this case two perturbative potential $V_{1,2}$ should be introduced. They have the form

$$V_0(r) = \sum_{G_0} (\eta^1(G_0) + \eta^2(G_0) + \eta^3(G_0))e^{iG_0\cdot r}.$$

(21)

FIG. 2. Square lattice with three alternating layers perpendicular to the selected diagonal in the real space (a) and its Brillouin zone (b). The unit cells of the simple square prophase and perturbative phase are shown by dashed and bold lines, respectively.
\[ V_{1,2}(r) = \sum_{\mathbf{k}_{\alpha}} \left[ \eta^1(\mathbf{G}_0 + \mathbf{Q}) - \eta^2(\mathbf{G}_0 + \mathbf{Q}) e^{-i\pi/3} - \eta^1(\mathbf{G}_0 + \mathbf{Q}) e^{i\pi/3} \right] \]

Here summing is over the reciprocal vectors of the simple square lattice \( \mathbf{G}_0 \). This time a new reciprocal vector \( \mathbf{Q} = (2\pi/3a)(1,1) \) is selected.

We note again that the prophase potential \( V_0 \) has the periodicity of the simple square lattice and satisfies the relation \( V_0(r+\mathbf{\tau}) = V_0(r) \), while for the perturbative potentials we have \( V_{1,2}(r+\mathbf{\tau}) = -V_{1,2}(r) e^{i\pi/3} \). The unit cell and Brillouin zone of the simple square prophase are shown in Fig. 2 by dashed lines. The area of the unit cell for the complex lattice with three alternating layers is greater than three times the area of the simple square lattice of the prophase, while the areas of the reciprocal unit cells, namely, the Brillouin zones, are characterized by the inverse relationship.

The perturbative analysis [Eqs. (13–18)] presented in Sec. II A for a lattice with two alternating layers can be easily extended to the lattice with three alternating layers. Now the matrix \( \tilde{\mathbf{R}}_{\mathbf{G}_0,\mathbf{Q}} \) will be a \( 3 \times 3 \) block matrix with diagonal blocks giving the band spectrum of the prophase in the points \( \mathbf{k}, \mathbf{k} + \mathbf{Q}, \) and \( \mathbf{k} - \mathbf{Q} \), interacting with each other through the potentials \( V_1 \) and \( V_2 \).

We can interpret the effect of including of the \( V_{1,2} \) potentials as triple folding of the simple square Brillouin zone. So that the spectrum of the perturbative phase along any direction \( M_1M_2 \) will be a sum of the three prophase branches: \( M_1M_2, \) \( (M_1 + \mathbf{Q})(M_2 + \mathbf{Q}) \) and \( (M_1 - \mathbf{Q})(M_2 - \mathbf{Q}) \). Here we define \( (M_1 \pm \mathbf{Q}) \) as a point inside the Brillouin zone with the coordinate \( (2\pi/3a)(x_1,y_1) \pm (2\pi/3a)(1,1) \), assuming that the coordinates of the point \( M \) are \( (2\pi/3a)(x_2,y_2) \). We conclude that the folding the Brillouin zone of the simple square lattice is governed by the vector \( \mathbf{Q} \) again, resulting in a strong mixing the states separated by this vector.

The developed model can be easily extended to the \( n \)-layer square lattice. In this case the prophase is determined by the simple square lattice again, but the folding reciprocal vector is given by \( \mathbf{Q} = (2\pi/na)(1,1) \). This results in interaction between the \( n \) plane wave states of the prophase \( [\mathbf{k}, \mathbf{k} \pm \mathbf{Q}, \ldots \mathbf{k} \pm (n-1)\mathbf{Q}] \) through \( n-1 \) perturbative potentials.

### III. PLANE WAVE CALCULATION

We proceed with this symmetrical consideration to analyze the plane wave calculations of the square lattice, shown in Figs. 1 and 2. In our numerical analysis, since the radius of the dielectric rods is a more flexible parameter, we have mostly paid attention to the case of varying radius of the rods, keeping the dielectric constants of the rods unchanged. A system of dielectric rods in air has been considered, with the dielectric constants of the rods \( \varepsilon_a = 11.9 \) and air \( \varepsilon_b = 1 \).

To calculate the band spectrum for the photonic crystals with a complex basis we followed the technique developed in Ref. 11. To obtain a faster convergence of the eigenvalue problem in our numerical calculations, we consider \( \eta^1(\mathbf{G} - \mathbf{G}') \) as a matrix found by inverting the matrix \( \varepsilon(\mathbf{G} - \mathbf{G}') \) defined by the Fourier transforms of the dielectric constant.\(^7,\^{17,18}\)

The results that follow were obtained using 569 plane waves for a simple square lattice with one rod in basis and 961 plane waves for the complex square lattices with alternating layers. A greater number of plane waves was required to maintain accuracy for the latter cases due to a more complex unit cell arrangement. The numerical data were tested using 1221 plane waves, showing that the accuracy of the results is better than 1%.

Figure 3 presents the plane wave band spectrum of the square photonic lattice with two alternating layers shown in Fig. 1, for the \( E \) polarization. Figures 3(a)–3(c) show the band spectrum for the cases of varying the radii of the rods and keeping their dielectric constant unchanged, namely, for the cases \( r_1 = r_2 = 0.2a \) (a), \( r_1 = 0.2a \) and \( r_2 = 0.21a \) (b), \( r_1 = 0.2a \) and \( r_2 = 0.3a \) (c). Figure 3(d) shows the band spectrum of alternating layers of dielectric rods with equal radii but different dielectric constants, namely, for the case \( \varepsilon_a^1 = 11.9 \) and \( \varepsilon_b^2 = 10 \). From the symmetrical analysis, we know that in the perturbative phase, the band spectrum along the \( \Gamma X' \) direction will be a sum of the two prophase branches from point \( 0 \) to \( (\pi/2a)(1,1) \) and from point \( (\pi/2a)(1,1) \) to \( (\pi/2a)(1,1) \), while the spectrum along \( \Gamma M' \) direction will be folded from the prophase spectrum along \( \Gamma X \) and \( M X \) directions.

At first, we note that Fig. 3(a) presents the band spectrum of the simple square lattice in the twice folded Brillouin zone. In the limits of the considered normalized frequencies, there are two points [labeled by the circles in Figs. 3(a), (3b) and (3d)] along \( \Gamma M' \) and \( \Gamma X' \) directions in which two bands of the prophase intersect. These bands are separated by the vector \( \mathbf{Q} = (\pi/a)(1,1) \). That is why they will have to split in the perturbative phase. Figures 3(b) and 3(c) clearly show how the band gap appears at these cross points and then increases with increasing \( r_2 \). An obvious reason for the opening of the band gap between fourth and fifth bands, labeled by the circles, is that these bands are related to the two different alternating layers perpendicular to the \( (11) \) direction. In support of this statement, in Fig. 4, we present the spatial distribution of the Poynting vector for the photonic crystal with \( r_1 = 0.2a, r_2 = 0.21a \) [Fig. 3(b)]. Figures 4(a) and 4(b), respectively, show the energy distribution for the fourth [\( \omega a/(2\pi c) = 0.489 \)] and the fifth [\( \omega a/(2\pi c) = 0.507 \)] bands at the labeled point in the \( \Gamma M' \) direction. In the prophase, all the layers are identical and the two bands have the same energy. However in the perturbative phase, the greater the difference between dielectric rods, the greater the energy splitting between these two bands [Fig. 3(c)].

Second, as follows from our symmetrical analysis, the band spectrum of the perturbative phase along the \( M'X' \) direction is folded by the two prophase bands from point \( \pi/a(1,1) \) to point \( \pi/2a(1,1) \) and from point \( \pi/2a(0, -1) \) to point \( \pi/a(0, -1) \). These bands are identical in the prophase [Fig. 3(a)], but when including the perturbation, the nondiagonal blocks in Eq. (17) split them into two bands (except some of the bands at the \( M' \) points which we discuss below). It is interesting to note that this splitting has an obvious support in the symmetry of the lattice. The vector \( M'X' \) in reciprocal space corresponds to the planes \{11\} in...
the real space which are identical in the prophase, but are of two different kinds in the perturbative phase. Third, we note that the symmetry of the lattice with two alternating layers is no less than the symmetry of the simple square lattice. That is why the degeneracy in the symmetrical points of the Brillouin zone still survives. This is the case for the points \( G \) and \( M \) of the Brillouin zone. The degeneracy at the \( G \) point cannot be lifted because the perturbative potential has the same symmetry \( C_4 \) as the small group symmetry of the \( G \) and \( M \) points of the prophase which generate the spectrum at the \( G \) point of the perturbative phase. The spectrum at the point \( M \) of the perturbative phase \(~\) with the \( C_2 \) small group symmetry \(~\) is the result of folding the spectrum at the \( X \) points of the prophase \(~\) with the \( C_2 \) small group symmetry. The states \( M_1 \) and \( M_2 \) are generated by the \( A_{1,2} \) one dimensional representations of the group \( C_{4v} \). They are obtained from the \( A_{1,2} \) representations of the small group \( C_{2v} \) of the points \( X \) of the prophase. When including the perturbation, they split into two bands resulting in the first \( E \)-band gap \([\text{Fig. 3(c)}]\). The small point group of the \( X' \) point is \( C_2 \). It includes only one-dimensional irreducible representations generating the nondegenerate states. That is why all states at the point \( X' \) are completely split by the perturbative potential. It is worth mentioning that the triple degeneracy of the \( \Gamma_{56} \) band is accidental. This is a result of the overlapping

FIG. 3. Plane wave band spectrum of the square photonic lattice with two alternating layers shown in Fig. 1 for \( E \) polarization in the cases \( \epsilon_1^a = 11.9, r_1 = 0.2 a \); \( \epsilon_2^a = 11.9, r_1 = 0.2 a \); \( \epsilon_2^a = 11.9, r_2 = 0.2 a \); \( \epsilon_1^a = 10, r_1 = r_2 = 0.2 \). The states are labeled in accordance with their ordering in the prophase.
between the nondegenerate and doubly degenerate bands, which appears already in the prophase and may be easily lifted by decreasing the radius of the second rod or by decreasing its dielectric constant.

The above analysis shows a qualitative agreement between the symmetrical model and the exact plane wave calculation of the band spectrum of the two layer crystals. In the case of small perturbation, it is easy to obtain a quantitative comparison between the data for the bands obtained in the frames of the standard plane wave model and the spectrum obtained from perturbative Hamiltonian (17). In the limit of the zero perturbation, nondiagonal blocks of Hamiltonian (17) equal to zero. That is why the exact and perturbative spectra completely overlap. In the perturbative phase, the most important issue is to compare magnitude of the band splitting at the points of removing the degeneracy. In the simplest approximation, we can take into account only the interaction between crossing bands. Then perturbative Hamiltonian (17) reduces to the $2 \times 2$ matrix. We easily obtain that, for small perturbations, the splitting of the bands at the $k$ point of the Brillouin zone is order of $\Delta E_k = |k + G_0| |k + G_0' + Q| \eta_{G_0 - G_0' - Q} / E_k^0$ (where $E_k^0$ is a normalized frequency for the treated band at the point $k$ in the prophase).

In the case of $r_1 = 0.2a$ and $r_2 = 0.21a$ [Fig. 3(b)], the direct estimation gives $\Delta E \sim 0.0173$ for the splitting of degenerate bands along $\Gamma M'$ direction [in this case $k = 2\pi/a(0.15,0)$, $G_0 = 2\pi/a(-1,0)$, $G_0' = 2\pi/a(-1,-1)$], while the exact solution for these bands gives $\Delta E = 0.018$. For the splitting of the $M_1'$ and $M_2'$ bands [at $k = \pi/a(1,0)$, $G_0 = G_0' = 0$], $\Delta E \sim 0.0059$, while the exact solution gives $\Delta = 0.0067$. We note that this rough estimation is in good agreement with the exact solution. This two-band approximation is valid only in the case if $|k + G_0| |k + G_0' + Q| \eta_{G_0 - G_0' - Q} < \delta E_k^0$. That is, if nondiagonal matrix element connecting two degenerate prophase states is less than the distance from the far bands.

**FIG. 4.** The space distribution of the Poynting vector, superimposed on the cylinder cross section, for the photonic crystal with $r_1 = 0.2a$, $r_2 = 0.21a$ [Fig. 3(b)] for the fourth (a) $(\omega a/(2\pi c) = 0.489)$ and fifth (b) $(\omega a/(2\pi c) = 0.507)$ bands at the label point on the $\Gamma M'$ direction.

**FIG. 5.** The space distribution of the Poynting vector, superimposed on the cylinder cross section, for the $M_34$ doubly degenerate state $(\omega a/(2\pi c) = 0.411)$ corresponding to the crystal shown in Fig. 3(b).
So, for the small perturbations, the two-band perturbative Hamiltonian gives very simple and reasonable estimation, but for large perturbations compared with the distance from far bands in the prophase, to obtain a good agreement with the \textit{ab initio} calculations a many-band model of perturbative Hamiltonian (17) has to be treated. In this case, the perturbative approach is missing its simplicity and standard plane wave calculations are more reasonable.

It is obvious that the effect of the different radii of the rods and different dielectric constants on the band spectrum should be similar in the photonic crystals studied. This is supported by a comparison of Fig. 3(b) and 3(c) and Fig. 3(d). That is why, in the results presented below, we restrict ourselves to varying radii of the rods, keeping the dielectric constants of the rods unchanged and equal to $\varepsilon_a = 11.9$.

The band spectrum for the $H$ polarization is shown in Fig. 6 in the cases $r_1 = r_2 = 0.2a$ (a), $r_1 = 0.2a$ and $r_2 = 0.21a$ (b), and $r_1 = 0.2a$ and $r_2 = 0.3a$ (c). At first we note from Fig. 6 that there are a few cross points, labeled by circles in the figure, in which the prophase states separated by the vector $Q$ intersect. But in this case, only the bands in the $\Gamma\chi'$ direction split, while the bands in the $\Gamma M'$ direction do not. To explain this we note, at first, that the intersection between the second and third $\Gamma M'$ bands appears already in the prophase and cannot be lifted by the highly symmetrical perturbative potential. As for the intersection between the third and fourth $\Gamma M'$ bands, it cannot be lifted because of the scalar product character of the matrix elements of the perturbative Hamiltonian for the $H$ bands that become equal to zero at these points on the $\Gamma M'$ axis. It is worth mentioning that this scalar product character of the eigenvalue Hamiltonian for the $H$ bands [Eq. (5)] results in much less splitting effect of the $H$ bands in comparison with the $E$ bands.

Second, we note that, for the $H$ polarization, the ordering of the doubly degenerate and nondegenerate states at the point $M'$ is reversed in comparison with the $E$ polarization (Fig. 3). Now the states $M'_{12}$ are generated by the two-dimensional representation of the group $C_{4v}$ and the states $M'_{34}$ and $M'_{56}$ by the one-dimensional representations. The
bands are labeled in accordance with their ordering in the prophase again. This effect was discussed in Ref. 15. It is related with the different symmetry of the \( E \) and \( H \) waves under reflection in the \( x\)-\( y \) plane.

Third, we note that the band spectrum of the photonic crystal with \( r_2 = 0.3a \) [Fig. 6(c)] shows a band gap with the middle point \( \sqrt{2}/(2\pi c) \approx 0.61 \). This band gap is very sensitive to the radius of the second rod. It appears only in the nearest neighborhood of the value \( r_2 = 0.3a \).

The plane wave calculations of a square lattice with three alternating layers are shown in Figs. 7 and 8. Figure 7 presents the plane wave band spectrum of the simple square photonic lattice for the \( E \) polarization with \( r = 0.2a \) in the three times folded Brillouin zone, shown by the bold lines in Fig. 2(b). The spectrum for the \( E \)-bands of the square lattice with \( r_1 = r_3 = 0.2a, \ r_2 = 0.2a \), and \( r_1 = r_3 = 0.2a, \ r_2 = 0.3a \) is shown in Figs. 7(b) and 7(c), respectively. As follows from Eq. (22), in this case the potentials \( V_1 \) and \( V_2 \) are similar.

At first, the \( C_2 \) group symmetry of this lattice is very low, and by symmetry all states lying on the boundary and in the symmetrical points of the Brillouin zone should be non-degenerate. If there is some degeneracy of the band spectrum of the prophase it must be lifted by the proper perturbation. We can follow in Fig. 7 how, including the perturbative potential, the band spectrum is generated from the spectrum of the prophase. In particular, the spectrum in the perturbative phase along the \( \Gamma T \) direction will be a sum of the three prophase branches: from point \( (0,0) \) to point \( (\pi/3a)(1,1) \), from point \( (2\pi/3a)(1,1) \) to point \( (\pi/a)(1,1) \), and from point \( -(2\pi/3a)(1,1) \) to point \( -(\pi/3a)(1,1) \). All the branches are different in the prophase spectrum. In the perturbative phase, the interaction of these branches must be most strong at the points of their intersection. As follows from Fig. 7 the band spectrum along the \( \Gamma T \) direction is the three times folded spectrum of the prophase. We note that the intersection between seventh and eighth \( \Gamma T \) bands, shown by the dashed circle, survives even for the large perturbative potential when the difference between the radii of the rods goes up to 10%. The numerical analysis shows that this degeneracy is accidental, and a band gap between these bands.
appears when \( r_2 < 0.2a \) (Fig. 8).

The spectrum of the perturbative phase along the \( \Gamma K \) direction will be a sum of the three prophase branches: from point \((0,0)\) to point \((2\pi/3a)(5/6, -5/6)\); from point \((2\pi/3a)(1,1)\) to point \((2\pi/3a)(11/6, 1/6)\); and from point \((2\pi/3a)(-1, -1)\) to point \((2\pi/3a)(-1/6, -11/6)\). But the last two branches are equivalent in the prophase. That is why, when including the perturbative potential, they will show splitting. We can follow the splitting of the equivalent second and third \( \Gamma K \) bands in the prophase marked by circles at the end points in Fig. 7(b) and 7(c). The figure clearly shows how the band gap appears at the intermediate points, between the circles on the \( \Gamma K \) branches and then increases with increasing \( r_2 \).

The spectrum of the perturbative phase along the \( \Gamma J \) direction is determined by the three prophase branches as well: from point \((0,0)\) to point \((2\pi/3a)(1, -1/2)\); from point \((2\pi/3a)(1,1)\) to point \((2\pi/3a)(2, 1/2)\); and from point \((2\pi/3a)(-1, -1)\) to point \((2\pi/3a)(0, -3/2)\). All three branches are not equivalent in the prophase. That is why the second and third \( \Gamma J \) bands do not overlap in the prophase; they have only two cross points, shown in circles. When including the perturbation they will split at the cross points. Similarly, we can follow the generation of the band gaps at the other intermediate points on the \( \Gamma J \) branches in Figs. 7(b) and 7(c) as well.

As the next step we study the change of the band spectrum when all the cylinders are different. In this case both potentials \( V_1 \) and \( V_2 \) are different, resulting in additional splitting of the band spectrum. Figure 8 shows the spectrum of the \( E \)-bands of the square lattice with \( r_1 = 0.2a, r_2 = 0.19a, r_3 = 0.3a \) (a); \( r_1 = 0.2a, r_2 = 0.15a, r_3 = 0.3a \) (b); and \( r_1 = 0.2a, r_2 = 0.1a, r_3 = 0.3a \) (c). We note that including the two different perturbative potentials \( V_1 \) and \( V_2 \) lifts the degeneracy of the spectrum further. Figure 8 shows how when decreasing the radius of the second rod from 0.2a to 0.1a, the band gap opens at the points \( P \) and \( K \) and then increases resulting in a complete \( E \)-band gap between the second and third bands.

From this analysis we arrive at the following conclusions.
The generation of the band spectrum in the perturbative phase goes in two steps. In the first step, the band spectrum of the prophase, governed by the corresponding vector \( Q \), is folded into the Brillouin zone of the perturbative phase. In the second step, the degeneracy of the band spectrum can be lifted by the perturbative potential. Whether it is lifted or not is directed by the symmetry of the perturbative potential. As an example, in the case of the square lattice with two alternating layers, the \( C_{4v} \) group symmetry of the perturbative potential lifts the degeneracy at the \( M'_{12} \) points (Fig. 3), but cannot completely lift the degeneracy at the points \( M'_{54}, M'_{56} \) and \( \Gamma_{34}, \Gamma_{56} \) of the Brillouin zone. The perturbative potential for the square lattice with three alternating layers has to satisfy the \( C_2 \) group symmetry; that is why all states on the boundaries of the Brillouin zone and at the symmetrical points should be nondegenerate.

IV. CONCLUSION

In this paper we have presented a symmetrical approach for analyzing the band spectrum of the complex photonic crystals. Our model allows us to select the simplest prophase with the most symmetrical spectrum, and then to follow the generation of the band spectrum of the complex photonic crystals when including the perturbative potentials. The generation of the band spectrum goes in two steps. In the first step, the band spectrum of the prophase, governed by the corresponding vector \( Q \), is folded into the Brillouin zone of the perturbative phase. In the second step, the degeneracy of the band spectrum is lifted by the perturbative potential. An important issue is that band gap can be opened both at the new boundaries of the Brillouin zone and inside of the Brillouin zone. In the framework of the developed model we can understand and predict the appearance of the band gaps of the crystals in question.

We have applied the results of the theoretical analysis to the plane wave calculations of the complex photonic crystals. The band spectrum of square photonic lattices with alternating layers perpendicular to the main square diagonal have been considered in some detail. Our analysis shows that the band spectrum of these photonic structures may be varied considerably by changing the parameters of the dielectric rods. Therefore, these photonic crystals form a wide class of tunable photonic structures. The theoretical results are in agreement with the ab initio numerical calculations of the band spectrum.

We emphasize that this approach is general. It may be used not only for analyzing many layer square crystals but for many layer hexagonal crystals and hexagonal comblike crystals, considered in Refs. 14 and 15. In the last case, the prophase is determined by a low symmetrical lattice, and two complex conjugate perturbative potentials transform it into the high symmetrical hexagonal lattice. We leave this intriguing problem for our next paper. To conclude, we believe that our analysis will be useful for understanding both the isolating and conducting properties of the photonic crystals, by a prediction of the points in the Brillouin zone where the band gap can be opened by some perturbation.

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