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A two-dimensional photonic crystal with six large bandgaps formed by a hexagonal lattice of anisotropic cylinders*

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The plane-wave expansion method is used to calculate the band structure of a two-dimensional photonic crystal formed by a hexagonal structure of anisotropic cylinders. Two cylindrical inclusions in the unit cell have two different radii, R_1 and R_2 ($R_1 < R_2$). By reducing the symmetry of the structure and choosing appropriately parameters R_2 and $s = R_1/R_2$ ($s < 1$), we obtain six large complete bandgaps, among which three are over 0.05 ω_e (where $\omega_e = \frac{2\pi c}{a}$) in the high region of the normalized frequency (however, one of these over 0.065 ω_e is not stable). There are two other stable complete bandgaps in the low-frequency region.

Keywords: complete bandgap, hexagonal structure, symmetry, stability
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In recent years, there has been a fast development in the research of photonic crystals, and much work has been done both theoretically and experimentally. A photonic crystal is a periodic arrangement of a dielectric medium or metal. If, in some frequency range, a photonic crystal reflects light of any polarization totally at any incident angle, the crystal is said to have an absolute photonic bandgap (PBG). Since electromagnetic waves with frequencies in the absolute gaps are totally forbidden, many potential applications in communications can be expected. It is thus important to design photonic crystals with large bandgaps. Although three-dimensional PBG structures may provide the most stirring potential in applications,[1−5] the fabrication of PBG structures is exceedingly difficult in the visible or infrared regime. In contrast, it is much easier to fabricate two-dimensional (2D) PBG structures in this regime and much attention has been drawn towards 2D PBG structures.[6−9] Furthermore, 2D structures could also find important applications such as reflective mirrors in laser diodes.[10]

An absolute PBG in a 2D case requires an overlap of the bandgaps for the E- and H-polarizations. It has been shown in previous work that degeneracy exists for simple cylinders in a 2D lattice.[4,11] Absolute bandgaps can be created by lifting the degeneracy. A natural way to lift the degeneracy is to reduce the symmetry of a photonic crystal. It is well known that symmetry reduction can remarkably increase the bandgaps of a photonic crystal. In general, there are three kinds of method to decrease the symmetry of a photonic crystal: (1) using an anisotropic material which has different refractive indices in the $x-y$ plane and the z-direction; (2) reducing the symmetry of the primitive lattice, such as replacing a square lattice with a rectangular lattice, or replacing a triangular lattice with a hexagonal structure; (3) reducing the symmetry of the inclusions inside the unit cell, such as replacing circular cylinders with elliptic cylinders. By decreasing the symmetry of a photonic crystal, one can obtain a larger PBG. For an anisotropic inclusion with ordinary refractive index n_o and extraordinary refractive index n_e, it is easy to match the relative positions of the bandgaps for the two modes to obtain complete bandgaps.[12,13] It is also known that a much larger PBG can be obtained when replacing cylinders with elliptic cylinders as inclusions.[14,15] If we use a photonic crystal with a triangle lattice of anisotropic

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elliptic cylinders, we can find a large bandgap (about 0.0449 ω_e) at high frequencies as well as a coexisting large absolute gap at low frequencies.[16] For a specific application, a photonic device works at a fixed frequency or in a fixed frequency range (e.g., a wavelength of about 1.55 μm is used in modern optical communications). On the other hand, it is known that it is easier to fabricate a photonic device with a larger size (i.e. with a large lattice constant a for a PBG device). Therefore, it is easier to fabricate a photonic crystal with an absolute bandgap occurring at the higher normalized frequency $\omega a/2\pi c$ (corresponding to a larger value of a), where ω is the frequency (fixed for a specific application), and c is the speed of light in vacuum. It is thus very important to investigate the PBG at high frequencies. Hexagonal structures are often used in 2D photonic crystals. Compared with a triangular structure, a hexagonal structure reduces the symmetry. We expect to obtain large bandgaps by using a photonic crystal with a hexagonal structure of anisotropic cylinders.

Many numerical simulation methods have been developed to calculate the band structure of a 2D photonic crystal. Among these are the plane-wave expansion method,[2-4] the finite difference time domain method (FDTD),[17-21] multiple-scattering theory,[22] the transfer matrix method,[23] and the finite-difference eigenvalue method,[24] etc.

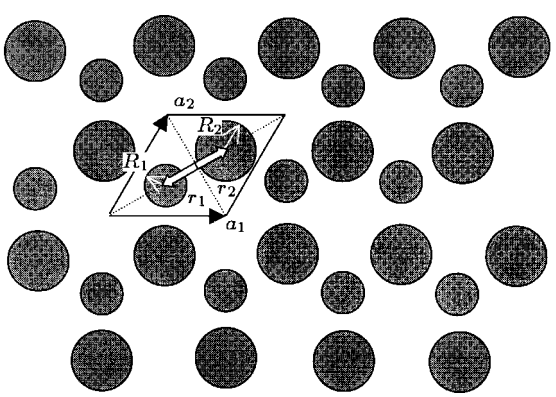


Fig.1. Geometric structure for a 2D hexagonal lattice of cylinders. $\mathbf{a_1}, \mathbf{a_2}$ are the basic vectors of the periodic parallelogram unit cell, and R_1 and R_2 are the radii of the two cylinders respectively. The centres of the two cylinders have been shifted by $\mathbf{r_1}$ and $\mathbf{r_2}$, respectively, from the centre of the unit cell.

In this paper, we use the plane-wave expansion method to calculate the bandgaps of a 2D photonic crystal with a hexagonal structure of anisotropic cylinders, aiming to obtain some large absolute PBG at a relatively high normalized frequency.

The 2D periodic structure that we consider is shown in Fig.1. This structure consists of two cylindrical inclusions with different radii R_1 and R_2 ($R_1 < R_2$) in a parallelogram unit cell.

In a 2D photonic crystal, we use the standard plane-wave expansion method to calculate the bandgap of a 2D photonic crystal with a hexagonal structure of anisotropic cylinders.[11] It is assumed that the cylindrical axis is along the z-direction and the 2D periodic structure is arranged in the $x-y$ plane. Two sets of cylinders (having different radii R_1 and R_2) with triangular lattices are arranged to form the hexagonal structure, in which the centres of one set of cylinders are located in the circumcircle centres of the other set of cylindrical triangular lattice. Thus we can choose the unit cell of the photonic crystal as follows: setting the lattice constant as a, basic vectors of the unit cell $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$, and the angle between $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ is 60°. Along the long diagonal of the parallelogram unit cell, two different cylinders are placed at $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$, respectively, with $\boldsymbol{r}_1$=-($\boldsymbol{a}_1$+$\boldsymbol{a}_2$)/6, $\boldsymbol{r}_2$=($\boldsymbol{a}_1$+$\boldsymbol{a}_2$)/6. The structure is shown in Fig.1.

Tellurium is an anisotropic material that has n_e=6.2 and n_o=4.8. We set $\epsilon_1(\boldsymbol{x}_\parallel)$=$\epsilon_2(\boldsymbol{x}_\parallel)$=$\epsilon_o(\boldsymbol{x}_\parallel)$=$n_o^2$, and $\epsilon_3(\boldsymbol{x}_\parallel)$=$\epsilon_e(\boldsymbol{x}_\parallel)$=$n_e^2$.

For H-polarization, we can obtain the following equation for the H_3 component:

$$\frac{\partial}{\partial x_1}\left[\frac{1}{\epsilon_o(\boldsymbol{x}_\parallel)}\frac{\partial H_3}{\partial x_1}\right] + \frac{\partial}{\partial x_2}\left[\frac{1}{\epsilon_o(\boldsymbol{x}_\parallel)}\frac{\partial H_3}{\partial x_2}\right] + \frac{\omega^2}{c^2}H_3 = 0, \qquad (1)$$

where c is the velocity of light in vacuum.

For E-polarization, one has the following equation for the E_3 component

$$\frac{1}{\epsilon_e(\boldsymbol{x}_\parallel)}\left[\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}\right]E_3 + \frac{\omega^2}{c^2}E_3 = 0. \qquad (2)$$

We expand $\dfrac{1}{\epsilon_{o,e}(\boldsymbol{x}_\parallel)}$, $H_3(\boldsymbol{x}_\parallel)$, and $E_3(\boldsymbol{x}_\parallel)$ according to

$$\frac{1}{\epsilon_{o,e}(\boldsymbol{x}_\parallel)} = \sum_{G_\parallel} K_{o,e}(\boldsymbol{G}_\parallel)e^{i(G_\parallel\cdot\boldsymbol{x}_\parallel)}, \qquad (3)$$

$$H_3(\boldsymbol{x}_\parallel) = \sum_{G_\parallel} \boldsymbol{A}(\boldsymbol{k}_\parallel \mid \boldsymbol{G}_\parallel)e^{i(G_\parallel+\boldsymbol{k}_\parallel)\cdot\boldsymbol{x}_\parallel}, \qquad (4)$$

$$E_3(\boldsymbol{x}_\parallel) = \sum_{G_\parallel} \boldsymbol{B}(\boldsymbol{k}_\parallel \mid \boldsymbol{G}_\parallel)e^{i(G_\parallel+\boldsymbol{k}_\parallel)\cdot\boldsymbol{x}_\parallel}, \qquad (5)$$

where $\boldsymbol{k}_{\parallel} = k_1\vec{e}_1 + k_2\vec{e}_2$ is the 2D wave vector in the x_1x_2 plane, and $\boldsymbol{G}_{\parallel} = \boldsymbol{G}_{m,n} = m\boldsymbol{b}_1 + n\boldsymbol{b}_2$

$$\begin{cases} \boldsymbol{b}_1 = \dfrac{2\pi}{a_c}(a_2^{(2)}, -a_1^{(2)}), \\ \boldsymbol{b}_2 = \dfrac{2\pi}{a_c}(-a_2^{(1)}, a_1^{(1)}), \end{cases} \tag{6}$$

where $a_j^{(i)}$ is the jth Cartesian component of the lattice vector $\boldsymbol{a}_i$, $a_c = \sqrt{3}a^2/2$ is the area of the unit cell, and m and n are integers.

Substituting these expansions into Eqs.(1) and (2), we obtain the following equations for the coefficients $\boldsymbol{A}(\boldsymbol{k}_{\parallel} \mid \boldsymbol{G}_{\parallel})$ and $\boldsymbol{B}(\boldsymbol{k}_{\parallel} \mid \boldsymbol{G}_{\parallel})$,

$$\sum_{G'_{\parallel}} (\boldsymbol{G}_{\parallel} + \boldsymbol{k}_{\parallel}) \cdot (\boldsymbol{G}'_{\parallel} + \boldsymbol{k}_{\parallel}) K_o(G_{\parallel} - G'_{\parallel}) A(\boldsymbol{k}_{\parallel} \mid \boldsymbol{G}'_{\parallel}) = \frac{\omega^2}{c^2} \boldsymbol{A}(\boldsymbol{k}_{\parallel} \mid \boldsymbol{G}_{\parallel}), \tag{7}$$

$$\sum_{G'_{\parallel}} |\boldsymbol{G}_{\parallel} + \boldsymbol{k}_{\parallel}||\boldsymbol{G}'_{\parallel} + \boldsymbol{k}_{\parallel}| K_e(\boldsymbol{G}_{\parallel} - G'_{\parallel}) B(\boldsymbol{k}_{\parallel} \mid \boldsymbol{G}'_{\parallel}) = \frac{\omega^2}{c^2} \boldsymbol{B}(\boldsymbol{k}_{\parallel} \mid \boldsymbol{G}_{\parallel}). \tag{8}$$

Fourier coefficients $K_{o,e}(\boldsymbol{G}_{\parallel})$ of $\epsilon_{o,e}^{-1}(\boldsymbol{x}_{\parallel})$ play a central role in the determination of the photonic band structures for both polarizations.

Since the centres of the two cylinders have been shifted from the centre of the unit cell by $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$, respectively, along the long diagonal, the Fourier coefficients have the following expression:[11]

$$K_{o,e}(\boldsymbol{G}_{m,n}) = \begin{cases} \varepsilon_{o,e}^{-1} f + (1-f), & \boldsymbol{G}_{m,n} = 0, \\ (\varepsilon_{o,e}^{-1} - 1)\dfrac{s^2 f}{1+s^2} J^{(1)} \exp\left(-i\dfrac{\pi}{3}(m+n)\right) + (\varepsilon_{o,e}^{-1} - 1)\dfrac{f}{+s^2} J^{(2)} \exp\left(i\dfrac{\pi}{3}(m+n)\right), & \boldsymbol{G}_{m,n} \neq 0, \end{cases} \tag{9}$$

where $J^{(i)} = \dfrac{2J_1(GR_i)}{GR_i}$, i=1,2, $J_1(x)$ is the Bessel function, G is the absolute value of vector $\boldsymbol{G}_{m,n}$, $f = \dfrac{\pi(R_1^2 + R_2^2)}{a_c}$ is the filling fraction, and $s = R_1/R_2$ $(s < 1)$.

As special cases of the structure, one can see that s=0 corresponds to a triangular structure, s=1 gives a honeycomb structure, and $0 < s < 1$ corresponds to a hexagonal structure. In order to verify our numerical code, we calculate the band structure for H-polarization with $\epsilon_e = \epsilon_o = 11.4$, $f = 0.431$, and $s = 0$. The calculated result is illustrated in Fig.2, which fits the result of Ref.[11] very well. In the case of a hexagonal structure $(0 < s < 1)$, from Fig.1 and Eq.(9) one sees that the four parameters (R_1, R_2, f and s) will influence the calculated result of the PBG. Since $f = \dfrac{\pi(R_1^2 + R_2^2)}{a_c}$ and $s = R_1/R_2$, there are only two independent parameters. In this paper, R_2 and s are chosen as parameters to be optimized. We use 961 plane waves, and the computational error is estimated to be less than 1% for the lowest ten photonic bands.

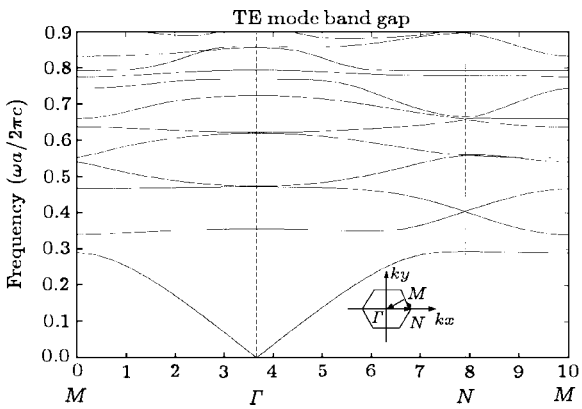


Fig.2. Band structure for a special case when s=0 (corresponding to a triangular structure) and ϵ_e=ϵ_o=11.4, f=0.431, for H-polarization. The band structure fits the result of Ref.[11] very well.

From Fig.1, one can see that the maximal value of R_2 is $\sqrt{3}a/6$. Thus we change s from 0 to 1, and R_2 from 0 to $\sqrt{3}a/6$ in order to search for the optimal parameters. By choosing appropriately parameters R_2 and $s = R_1/R_2$ $(s < 1)$, six large complete bandgaps appear. We number these bandgaps by starting from the lowest central frequency. As mentioned before, a bandgap at high frequencies has a practical significance. In the present paper, we have carefully calculated the bandgap at high frequencies, and the results for the six bandgaps are given in Table 1. At high frequencies there are three complete bandgaps. In the process of fabricating a photonic crystal, error is inevitable. Thus, it is necessary to discuss the stability of the optimal parameters. Bandgap 5 is large, and there are two optimal sets of parameters for this band. The optimal results for this bandgap are illustrated in Figs.3(a) and (b). From Fig.3(a), we can find that the bandgap reaches the maximum value of about 0.057 ω_e when R_2=0.176a and s=0.744. From Fig.3(b), one sees that the maximum value of the bandgap is about

0.052 ω_e when R_2=0.214a and s=0.78. The calculated result of bandgap 6 is illustrated in Fig.4, from which one sees that the maximum value of the bandgap is about 0.043 ω_e when R_2=0.194a and s=0.688. These bandgaps are stable under any parameter perturbation. Bandgap 4 can reach a maximum value of about 0.065 ω_e; however, this bandgap is not stable.

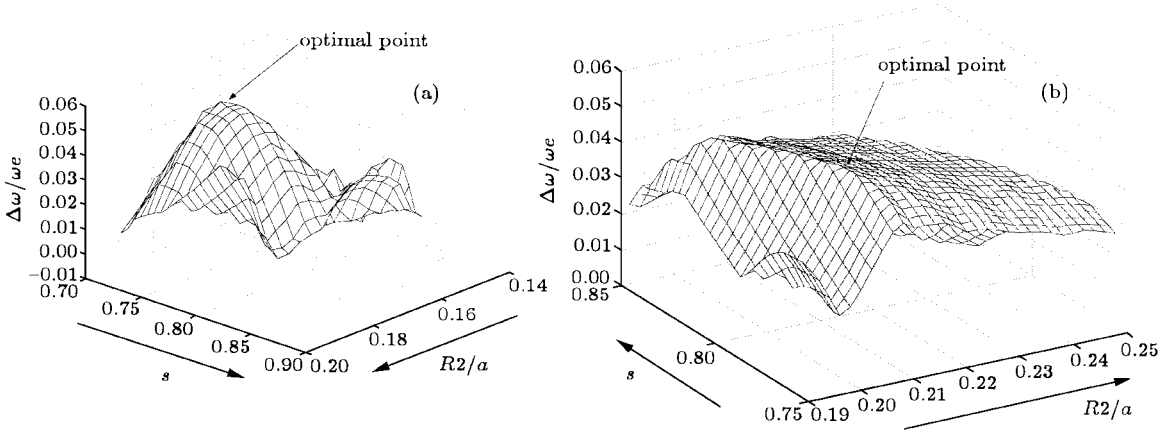


Fig.3. Optimization result for bandgap 5. (a) The maximum bandgap is 0.057 ω_e when R_2=0.176a and s=0.744. (b) The maximum (locally) bandgap is 0.052 ω_e when R_2=0.214a and s=0.78.

Table 1. Optimization results for the six bandgaps.

Bandgap number	R_2 (a)	s	Maximal bandgap (ω_e)	Central frequency (ω_e)
1	0.215	0.750	0.0375	0.03875
2	0.165	0.750	0.0275	0.5462
3	0.210	0.785	0.0549	0.5642
4	0.142	0.715	0.065	0.9281
5	0.176	0.744	0.057	0.9638
5	0.214	0.780	0.052	0.9308
6	0.194	0.688	0.043	1.077

In summary, the plane-wave expansion method has been employed to calculate the band structure of a 2D photonic crystal formed by a hexagonal lattice of tellurium elliptic cylinders. After optimizing the parameters R_2 and $s = R_1/R_2$ ($s < 1$), we have obtained six large complete bandgaps, among which three are over 0.05 ω_e in the high region of the normalized frequency (however, one of these over 0.065 ω_e is not stable). There are two other stable complete bandgaps in the low-frequency region. The stability of the designed parameters under any parameter perturbation has been checked carefully.

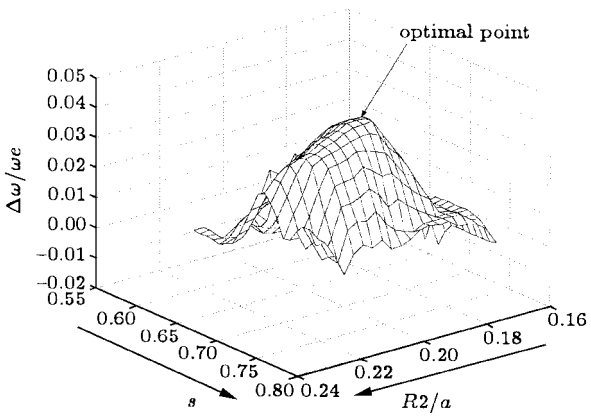


Fig.4. Optimization result for bandgap 6. The maximum bandgap is 0.043 ω_e when R_2=0.194a and s=0.688.

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