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Photonic band gaps of polygonal and circular dielectric rods in square lattices

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The plane-wave method is employed to determine the band structures and the field patterns of the photonic crystals with polygonal and circular rods in square lattices. Isotropic and anisotropic N -fold polygonal rods are used to assess the effects of the shapes and symmetries of polygonal rods on E - and H -polarization modes. The photonic band structures of the polygonal rods approach those of the circular rods as N increases above a value that is determined by the optical properties of the photonic crystal. Moreover, for comparable geometric structures, anisotropic polygonal-rod photonic crystals can provide larger absolute photonic band gaps than isotropic photonic crystals. © 2008 American Institute of Physics. [DOI: 10.1063/1.3039213]

I. INTRODUCTION

In recent years, photonic crystals have attracted much attention because of their various interesting properties and many innovative applications.¹⁻⁵ Various crystal structures with absolute photonic band gaps (PBGs), in which photons within a particular frequency range cannot propagate in the crystals, have been developed.^{1,6-8}

Many applications require large absolute PBGs. They include optical waveguides, defect cavities, and photonic crystal fibers.⁹⁻¹¹ Several attempts have been made to produce photonic crystals with large PBGs, including increasing the difference between the refractive indices of the rods and the background, trimming the rods, and tuning the filling factor.¹²⁻¹⁶ Photonic crystals have been constructed with solidified dielectric or void rods in square, hexagonal, and triangular lattices. Square dielectric rods in a square lattice, but not circular dielectric rods therein, exhibit absolute PBGs,^{17,18} suggesting that the shapes or the symmetries of rods may strongly influence the band structures of the dielectric rods in square lattices.

To demonstrate this proposition, the symmetries of N -fold polygonal rods are augmented up to those of circular rods in square lattices under a fixed filling factor and their band structures are calculated using the plane-wave method. The effects of symmetry of the isotropic polygonal rods, in terms of the side number N , on the E - and H -polarization band structures are investigated.

Absolute PBGs can be developed using anisotropic rods, by taking advantage of the tunability of the E - and H -polarization band gaps, which enables them to overlap each other.^{19,20} Following these developments, N -fold polygonal and circular anisotropic tellurium (Te) rods are constructed with the same filling factor, and their band structures are calculated to identify large absolute PBGs in these pho-

tonic crystals. The effects of the structural symmetries on the E - and H -polarization band structures of anisotropic polygonal rods are examined and discussed.

II. THEORY

Photonic band structures can be obtained by solving Maxwell's equations. In a source-free, time-invariant, and nonpermeable ($\mu = \mu_0$) space, Maxwell's equations can be written in terms of a magnetic field as a master equation,

$$\nabla \times \left[\frac{1}{\epsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) \right] = \frac{\omega^2}{c^2} \mathbf{H}(\mathbf{r}), \quad (1)$$

where $\mathbf{H}(\mathbf{r})$ is the magnetic field, $\epsilon(\mathbf{r})$ is a position-dependent dielectric constant, ω is the angular frequency, and c is the speed of light *in vacuo*. For periodic systems, the magnetic field $\mathbf{H}(\mathbf{r})$ and the dielectric function $\epsilon(\mathbf{r})$ can be expressed as sums of plane waves,

$$\mathbf{H}(\mathbf{r}) = \sum_{\mathbf{G}} \sum_{\lambda=1,2} h_{\mathbf{G},\lambda} \hat{e}_{\lambda} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} \quad (2)$$

and

$$\epsilon(\mathbf{r}) = \sum_{\mathbf{G}} \epsilon(\mathbf{G}) e^{i\mathbf{G}\cdot\mathbf{r}}, \quad (3)$$

where $h_{\mathbf{G},\lambda}$ is the coefficient of the \mathbf{H} component, \mathbf{k} is the wave vector in the Brillouin zone, and \mathbf{G} is the reciprocal-lattice vector. Two independent polarizations characterized by the unit vectors $\hat{e}_{\lambda} (\lambda=1,2)$ are perpendicular to the propagation vector $(\mathbf{k}+\mathbf{G})$. Under Fourier transform, the coefficient $\epsilon(\mathbf{G})$ is defined as

$$\epsilon(\mathbf{G}) = \frac{1}{A_{\text{cell}}} \int_{\text{cell}} \epsilon(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} d\mathbf{r}, \quad (4)$$

where A_{cell} is the area of the primitive cell of the lattice. Therefore, Eq. (1) can be expressed in matrix form,

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$$\sum_{\mathbf{G}'} |\mathbf{k} + \mathbf{G}| |\mathbf{k} + \mathbf{G}'| \begin{bmatrix} \varepsilon_{\mathbf{G},\mathbf{G}'}^{-1}(\hat{e}_2 \cdot \hat{e}'_2) & -\varepsilon_{\mathbf{G},\mathbf{G}'}^{-1}(\hat{e}_2 \cdot \hat{e}'_1) \\ -\varepsilon_{\mathbf{G},\mathbf{G}'}^{-1}(\hat{e}_1 \cdot \hat{e}'_2) & \varepsilon_{\mathbf{G},\mathbf{G}'}^{-1}(\hat{e}_1 \cdot \hat{e}'_1) \end{bmatrix} \times \begin{bmatrix} h_{1,\mathbf{G}'} \\ h_{2,\mathbf{G}'} \end{bmatrix} = \frac{\omega^2}{c^2} \begin{bmatrix} h_{1,\mathbf{G}} \\ h_{2,\mathbf{G}} \end{bmatrix}, \quad (5)$$

where $\varepsilon_{\mathbf{G},\mathbf{G}'}^{-1} = \varepsilon^{-1}(\mathbf{G} - \mathbf{G}')$ is the inverse of the matrix $\varepsilon(\mathbf{G} - \mathbf{G}')$. Eigenvalue (5) can be solved using the matrix diagonalization approach.

The axes of anisotropic dielectric rods with ordinary refractive index n_o and extraordinary refractive index n_e are parallel to the extraordinary axis. The refractive index is n_e for the E -polarization mode when the electric field vector is parallel to the extraordinary axis and becomes n_o for the H -polarization mode when the electric field vector is perpendicular to the extraordinary axis. The calculations pertain only to the case in which the wave vectors of the eigenmodes lie on the x - y plane and are uniform in the z -direction. The dielectric constant is given by

$$S(\mathbf{G}) = \begin{cases} \sum_{j=1}^N \frac{i\Delta y_j e^{-i\mathbf{G} \cdot \mathbf{C}_j} \sin(\mathbf{G} \cdot \mathbf{S}_j)}{G_x \mathbf{G} \cdot \mathbf{S}_j} & \text{for } G_y = 0 \\ \sum_{j=1}^N \frac{-i\Delta x_j e^{-i\mathbf{G} \cdot \mathbf{C}_j} \sin(\mathbf{G} \cdot \mathbf{S}_j)}{G_y \mathbf{G} \cdot \mathbf{S}_j} & \text{for } G_x = 0 \\ \sum_{j=1}^N \frac{2i\hat{e}_z(\mathbf{G} \times \mathbf{S}_j) e^{-i\mathbf{G} \cdot \mathbf{C}_j} \sin(\mathbf{G} \cdot \mathbf{S}_j)}{G^2 \mathbf{G} \cdot \mathbf{S}_j} & \text{for } G_x \neq 0, G_y \neq 0, \end{cases} \quad (9)$$

where $\mathbf{C}_j \equiv (\mathbf{P}_{j+1} + \mathbf{P}_j)/2$ and $\mathbf{S}_j \equiv (\mathbf{P}_{j+1} - \mathbf{P}_j)/2$ and $\Delta x \equiv x_{j+1} - x_j$ and $\Delta y \equiv y_{j+1} - y_j$.

The band structures of these photonic crystals are calculated using a standard plane-wave method. The calculations for the anisotropic photonic crystals are performed in the same way as for the isotropic photonic crystals. This work uses 841 plane waves, and the computational errors for the E - and H -polarization modes were estimated to be under 1% in all cases.

III. RESULTS AND DISCUSSION

In this study, the photonic crystals comprise isotropic and anisotropic circular and N -fold polygonal rods in square lattices. For isotropic photonic crystals, the dielectric constant of rods is set to 12.9, which is the dielectric constant of GaAs at 1.55 μm . The background is air with a dielectric constant $\varepsilon_b = 1.0$. A filling factor $f = 0.45$ is chosen for all photonic crystals, a value which is optimal for the isotropic square rods in the square lattice, as determined by our preliminary evaluation. The band structures of such established

$$\varepsilon(\mathbf{r}) = \varepsilon_b + (\varepsilon_{e,o} - \varepsilon_b) S_{\text{rod}}(\mathbf{r}), \quad (6)$$

where $S_{\text{rod}}(\mathbf{r})$ is a function of the rods, and ε_e and ε_o are dielectric constants that correspond to the refractive indices n_e and n_o , respectively. Substituting Eq. (6) into Eq. (4) yields the Fourier coefficient,

$$\varepsilon(\mathbf{G}) = \begin{cases} \varepsilon_{e,o} f + \varepsilon_b(1-f) & \text{for } \mathbf{G} = 0 \\ (\varepsilon_{e,o} - \varepsilon_b) S(\mathbf{G}) & \text{elsewhere,} \end{cases} \quad (7)$$

where f is the filling factor, which is the ratio of the cross-sectional area of a rod to that of a primitive unit cell. The structure factor is given by $S(\mathbf{G}) = (1/A_{\text{cell}}) \int_{\text{rod}} e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}$. The structure factor of the circular rod is

$$S(\mathbf{G}) = \frac{2\pi r_a}{G} J_1(G r_a), \quad (8)$$

where G is the magnitude of \mathbf{G} , J_1 is the first-order Bessel function of the first kind, and r_a is the radius of the circular rod. N -fold equilateral polygonal rods with the j th vertex coordinate $\mathbf{P}_j = (x_j, y_j)$ are considered. According to Stokes' theorem, the structure factor of such a polygonal rod can be expressed as

polygonal-rod photonic crystals are determined by the value of N and the angle θ between the side of the polygon and the lattice basis vector.

Figures 1(a) and 1(b) present the side lengths and the radii of the inscribed circles, R_{inner} , and the radii of the circumcircles, R_{outer} , for N -fold equilateral polygons in units of the lattice constant a for $N=4$ to $N=20$. As shown in the figure, the side length varies negligibly with N above 12. As N approaches infinity, the side length becomes zero and R_{inner} equals R_{outer} . Figures 2(a) and 2(b) plot the photonic band structures of photonic crystals with isotropic circular rods ($N=\infty$) and square rods ($N=4$), respectively, for $\theta=0$ in square lattices. The dispersion curves are traced along the M - T - X - M - X' - T path in the first Brillouin zone of the square lattice. The solid curves represent E -polarization modes and the dotted curves represent H -polarization modes. As shown in Fig. 2(a), the circular rods in the square lattice do not have a large H -polarization band gap at frequencies under $\omega a/2\pi c$. This result indicates the absence of a feasible absolute PBG in the circular-rod photonic crystals. However as shown in Fig. 2(b), the square-rod photonic crystal holds a

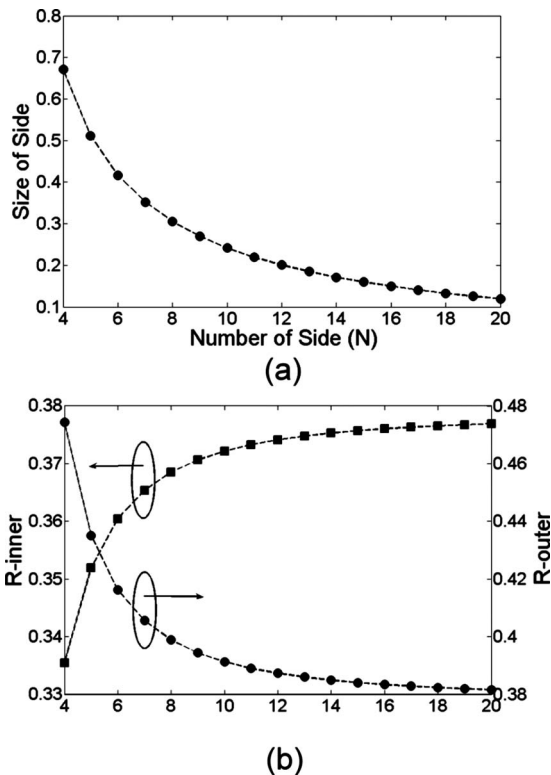


FIG. 1. (a) Lengths of sides and (b) radii of inscribed circles and circumcircles of N -sided equilateral polygons at a filling factor of 0.45 in units of lattice constant a .

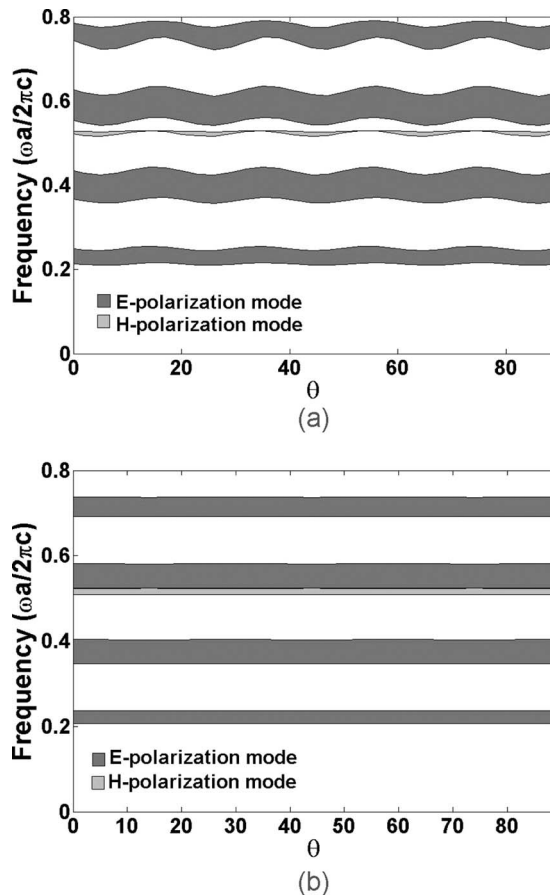


FIG. 3. PBGs of N -sided isotropic polygonal rods as function of rotation angle θ for (a) $N=9$ and (b) $N=12$.

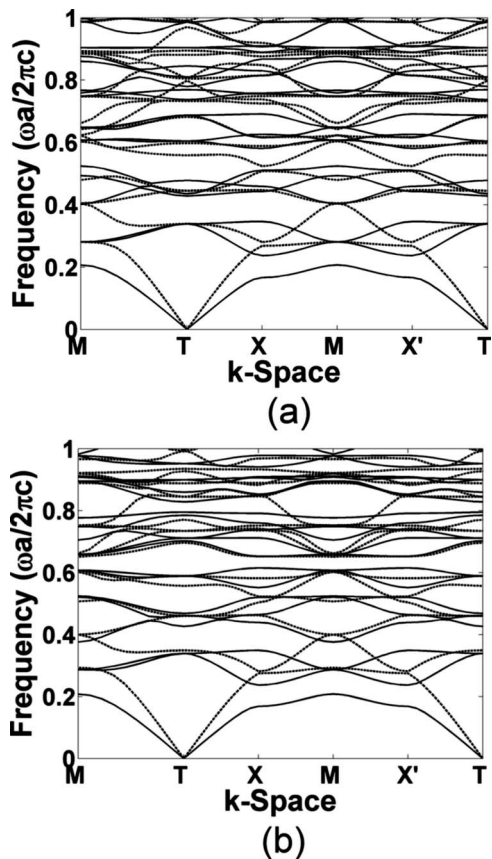


FIG. 2. Band structures of isotropic (a) circular dielectric rods and (b) square dielectric rods in square lattices, with a filling factor of 0.45.

sizable absolute PBG at high normalized frequency of around 0.62. Absolute PBG occurs in the region where the E_8 and H_6 (not designated in the figure) gaps overlap, where E_i or H_i represents the band gap between the i th and the $(i + 1)$ th bands of the E - or the H -polarization modes.

Figures 3(a) and 3(b) show the band gaps of 9-sided and 12-sided polygonal rods as a function of rod rotation angle θ for both polarization modes. For square lattices, these functions have a period of 90° . Only the bands below the 14th are considered here. The midgap positions of both polarization modes vary notably for the polygonal rods with an odd number of sides (such as $N=9$) and even more so for those with a smaller odd number of sides ($N=5$ and 7 ; not shown here). For polygonal rods with a large even number of sides (such as $N=12$), midgap positions remain almost constant as the rods rotate in a square lattice. The midgap positions of polygonal rods with a small even number of sides (such as $N=4$; not shown here) vary less than those of compatible polygonal rods with a small odd number of sides (such as $N=5$). These results are consistent with the variation in symmetry from small to large odd-/even-number-sided polygonal under rotation in square lattices.

Figure 4 presents the band gaps of polygonal rods ($N=4$ to $N=20$) and circular rods (at the right of the figure), at rotation angle $\theta=0$, for both polarization modes. For the E -polarization modes, five- and seven-sided polygonal rods do not have the same number of gaps as the other sided

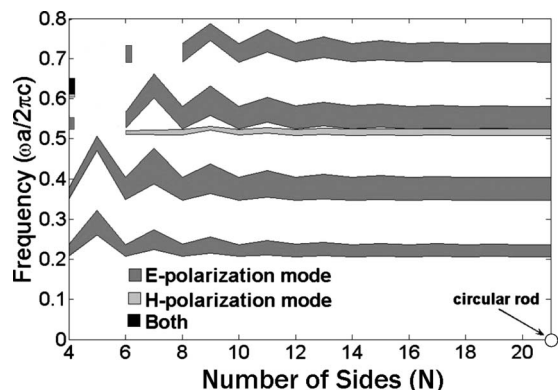


FIG. 4. PBGs of N -sided isotropic polygonal and circular rods as function of N .

polygonal rods. The high-frequency gaps of square and six-sided polygonal rods are specifically plotted in bars revealing the frequency ranges. It is observed that the midgap positions of the E -polarization modes are about the same for polygonal rods with an even number of sides but vary significantly for those with a small odd number of sides. The H -polarization gaps neither become wide nor overlap with the E -polarization gaps. The situation is similar when the angles of rotation are not zero. Consequently, no absolute PBG is available for these polygonal rods, except for the square rods.

In H -polarization modes, the electric field is oriented on the x - y plane and the tangential electric field is present in the low-dielectric background regions (air) to satisfy the boundary continuity. The electromagnetic interaction among the high-dielectric rods influences the proportion of field energy that is in the dielectric regions, and thus changes the band structures of H -polarization modes. As presented in Fig. 1(b), the radius of the circumcircle declines as N increases, indicating that the air space between the nearest rods becomes smaller as the number of sides of the rods declines. Therefore, the H -polarization bands shift drastically with N when N is small. In contrast, when N exceeds 10, the air space changes negligibly. The interaction between the fields influences the H -polarization bands in a comparable level and thereby insignificantly changes the H -polarization band gap. The gap-midgap ratio r is defined as the ratio of the gap width $\Delta\omega = \omega_U - \omega_D$ to the midgap frequency ω_0 , where ω_D and ω_U are the lower and upper band edge frequencies of the gap, respectively. The gap-midgap ratio is 0.045 for the H_6 gap of the circular rods. The difference between the gap-midgap ratios of the circular and polygonal structures is less than 0.01 when N is greater than 10.

In E -polarization modes, the proportion of field energy concentrated in the dielectric regions dominates the gap width and midgap frequency. The field patterns of the photonic crystals are adopted to evaluate the effect of the polygonal structures on the E -polarization modes. Figures 5(a)–5(h) display the field patterns of the polygonal structures with $N=4$ to $N=11$ sides and Fig. 5(i) displays the field pattern of the circular structure. These field patterns pertain to the E_8 band at the M -symmetry point. The E -polarization mode is related to the displacement field \mathbf{D} that is normal to

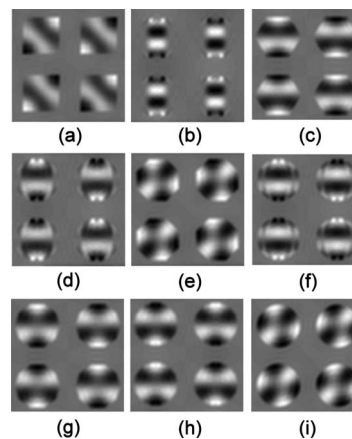


FIG. 5. Field patterns of E -polarization E_8 band at M -symmetry point in N -sided polygonal rods for $N=(a)$ 4, (b) 5, (c) 6, (d) 7, (e) 8, (f) 9, (g) 10, (h) 11, and (i) circular rods.

the x - y plane: $\mathbf{D}(\mathbf{r}) = d(\mathbf{r})\hat{e}_z$, where $d(\mathbf{r})$ is the magnitude of the displacement field. The displacement field is observably localized within the even- N -sided polygonal and circular rods. The E -polarization bands of the even-sided polygonal rods can be reasonably asserted to be analogous to those of the circular structures.

However, the displacement field is not distributed well within the dielectric rod regions of the odd- N polygonal structures—especially for $N=5$. The fraction of the field that is outside the dielectric regions indicates that E -polarization bands tend to move toward higher normalized frequencies, unlike in the case of even-sided polygonal structures. Additionally, the amplitude and the distribution of the displacement field in the dielectric polygonal rods approach those of the dielectric circular rods as N increases. The gap-midgap ratio is 0.148 for the E_8 gap of the circular structure. The difference between the gap-midgap ratios of the circular and polygonal structures is less than 0.01 when N exceeds 12. Figure 6 plots the band structure of the 12-sided polygonal-rod photonic crystal. The band structure of the 12-sided polygonal-rod photonic crystal is analogous to that of the circular-rod photonic crystal, as presented in Fig. 2(a), for both polarizations.

The convolution of the E -polarization and H -polarization band gaps in polygonal-rod photonic crystals reveals that the optical properties of N -fold polygonal rods in square lattices are the same as those of circular rods in square lattices when N exceeds 12. This fact is useful in designing and fabricating polygonal-rod photonic crystals.

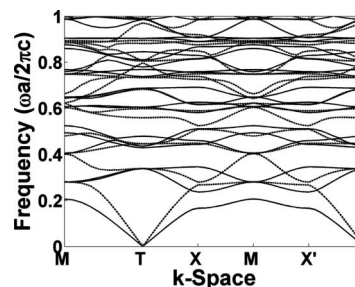


FIG. 6. Band structure of 12-sided isotropic polygonal rods in square lattice.

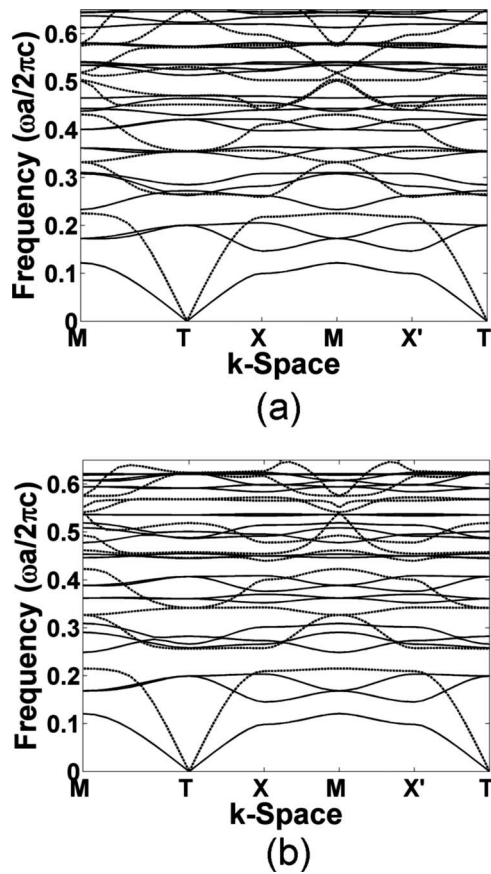


FIG. 7. Photonic band structures of anisotropic (a) circular rods and (b) square rods in square lattices, with a filling factor of 0.45.

Large absolute PBGs can be attained using dielectric rods of anisotropic materials.^{19,20} The gap width and the mid-gap position can be adjusted by varying the refractive index contrast. This study also investigates the photonic band structures of polygonal and circular Te rods in square lattices. Te is an anisotropic optical material with extraordinary refractive index $n_e=6.2$ and ordinary refractive index $n_o=4.8$ at wavelengths between 3.5 and 14 μm .^{20,21} The absorption coefficient of Te in the infrared region is less than 1 cm^{-1} .²² The refractive indices and the absorption coefficient of Te depend on frequency.²⁰⁻²² Our preliminary calculations verified that, based on the assumption that the refractive indices of Te are constant and the negligibility of the effect of absorption on the structures, no noticeable error occurs when the frequency is in an appropriate range and the structures are of a finite size.

Figures 7(a) and 7(b) show the photonic band structures of Te circular and square rods, respectively, in square lattices at a filling factor of 0.45. The photonic band structures of Te circular rods have two large absolute PBGs. However, the square rods have no feasible absolute PBG. Figure 8 presents the band gaps of Te polygonal rods for $N=4$ to $N=20$ and circular rods (at the right of the figure) for both polarization modes. Five- and seven-sided polygonal rods do not have as many gaps as the other sided polygonal rods in E -polarization modes. The high-frequency gaps of square and six-sided polygonal rods are highlighted with bars revealing their frequency locations. The refractive indices as-

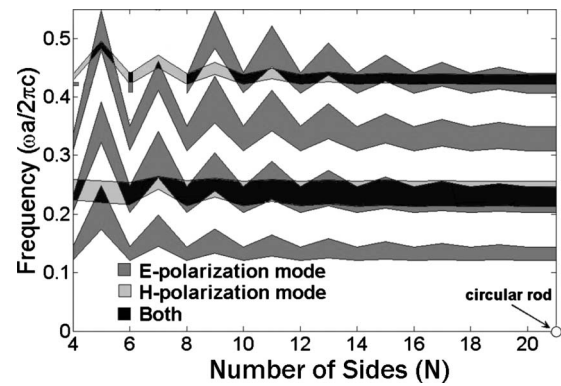


FIG. 8. PBGs of anisotropic rods as function of N .

sociated with E - and H -polarization modes of Te are larger than the refractive index of the isotropic material, considered above. The overall bands of the E -polarization and H -polarization modes tend to move toward lower frequencies than those in the cases of isotropic structures, as presented in Fig. 4. In particular, the H -polarization gap is sizable for each N and overlaps well with the E -polarization gap. Hence, the photonic crystals with anisotropic Te rods have large absolute PBGs.

In the H -polarization modes of Te rods, the difference between the gap-midgap ratios of the circular and polygonal rods is less than 1% for $N \geq 10$. The variation in the H -polarization bands on the number of sides of the polygon, N , can be analyzed in a manner similar to that in the isotropic cases. However, the E -polarization bands of the anisotropic structures are more sensitive to the number of sides, N , than are those of the isotropic structures. The gap-midgap ratio for the E_3 gap of the circular structure is 0.175. The difference between the gap-midgap ratios of the N -sided polygonal structures and the circular structures is less than 0.01 when N is greater than 18. The band structures clearly depend strongly on the shape and the boundaries of the polygonal rods when the photonic crystals are formed from anisotropic material. Hence, the requirements for fabricating anisotropic photonic crystals are stricter than those for fabricating isotropic photonic crystals.

IV. CONCLUSION

In this work, the band structures and the field patterns of polygonal- and circular-rod photonic crystals are calculated using the plane-wave method. The effects of polygonal structures on E - and H -polarization modes are investigated. The anisotropic polygonal-rod photonic crystals can provide a larger absolute PBG than the isotropic ones. For an isotropic material with refractive index $n=3.59$ ($=\sqrt{12.9}$), the band structure of the N -fold polygonal rods approaches that of circular rods as N increases above 12. In the case of anisotropic material with extraordinary refractive index $n_e=6.2$ and ordinary refractive index $n_o=4.8$, the band structure of N -sided polygonal rods resembles that of the circular rods when N exceeds 18. Moreover, the E -polarization bands of the anisotropic photonic crystals are more sensitive to the structural symmetry of the rod than are those of the isotropic

photonic crystals. These results guide the designing and fabrication of photonic crystals with polygonal rods in square lattices.

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