Large Absolute Band Gap in 2D Anisotropic Photonic Crystals

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Absolute photonic band gaps can be substantially improved in two-dimensional square and triangular lattices of cylinders by introducing anisotropy in material dielectricity. Owing to different refractive indices for electromagnetic waves with E and H polarization, the band gaps for the two polarization modes can be freely adjusted and matched to overlap optimally. Large absolute band gaps can be created for uniaxial cylinders in air with a positive anisotropy. In the case of air holes in background uniaxial dielectric with even a weak negative anisotropy, the absolute band gap can be increased 2–3 times. [S0031-9007(98)07161-0]

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In recent years there appears great interest in fabricating the photonic band gaps (PBG) structure, which exhibits a "forbidden" frequency region where electromagnetic waves cannot propagate for both polarizations along any directions [1,2]. This may bring about some peculiar physical phenomena [3–7], as well as wide applications in several scientific and technical areas [1,2]. Although three-dimensional (3D) PBG structures will provide the most stirring potential in applications, the fabrication of such PBG structures with a band gap in the visible or infrared regime is exceedingly difficult. In contrast, it is much easier to fabricate two-dimensional (2D) PBG structures in this regime [8–11]. Furthermore, 2D structures could also find some important uses such as a feedback mirror in laser diodes [12]. Perhaps for this reason, much attention has been drawn towards 2D PBG structures.

Since the superior features of PBG structures result from the photonic band gap, it is essential to design crystal structures with a band gap as large as possible. It is well known that the electromagnetic wave can be decomposed into the E- and H-polarization modes for a 2D structure. An absolute band gap exists for a 2D PBG crystal only when band gaps in both polarization modes are present and they overlap each other. Thus it is our aim to search for some structures with an optimal overlapping band gap by varying parameters of the photonic crystal, such as lattice type, refractive index contrast, filling fraction, and atom configurations.

It has recently been reported that the symmetry reduction of atom configuration by introducing a two-point basis set in simple 2D lattices can remarkably increase absolute band gaps [13], quite similar to the 3D case for diamond structures [14]. Very recently, it was found that the anisotropy in atom dielectricity can also break the degeneracy of photonic bands such that partial band gaps can be created in fcc, bcc, and simple cubic lattices [15]. In this Letter, we will demonstrate that such an anisotropy in dielectricity can remarkably increase absolute band gaps in 2D PBG structures.

The photonic band structure is left determined by the refractive index contrast, provided that other parameters such as lattice type, filling fraction, and atom configuration are fixed. The sizes and positions of band gaps can be adjusted by varying the refractive index contrast. Thus, if we choose different refractive index contrasts for the E- and H-polarization modes in a given photonic crystal, we can match the relative position of band gaps for the two modes. This will enable the optimal overlapping of band gaps and the largest absolute band gap can be obtained. One way available is to fabricate photonic crystals from materials with anisotropy in dielectricity. Nature offers a lot of anisotropic crystals which are lossless and transparent in visible or infrared regime. Among them are uniaxial crystals, which have two different principal refractive indices known as ordinary refractive index n_o and extraordinary refractive index n_e.

For simplicity and not without generality, we prefer to choose the extraordinary axis of uniaxial crystal parallel to the extension direction of cylinders. Then Maxwell's equations for such an anisotropic 2D PBG structure can be decomposed into two equations satisfied by the E- and H-polarization modes, respectively. They are the same as in the case of isotropic PBG structures, except that the dielectric constants for the two modes are now different. As the electric field vector in the E-polarization mode is parallel to the extraordinary axis, while perpendicular to the extraordinary axis in the H-polarization mode, the refractive indices are n_e and n_o for the E- and H-polarization modes, respectively.

The anisotropic photonic band structures are calculated using the plane-wave expansion method [14–16], which is also the same as in the case of isotropic photonic

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crystals. The results were obtained using 289 plane waves. The convergence accuracy for the several lowest photonic bands is better than 1%.

We first examine 2D photonic crystals consisting of dielectric cylinders in air. The cylinders are arranged in triangular lattice. The photonic properties of isotropic structures have been studied and shown to exhibit band gaps for each of the two polarization modes [16]. However, there is some discrepancy about whether an absolute band gap is present. Our simulations demonstrate that band gaps in the two polarization modes do not overlap with each other, resulting in the absence of the absolute band gap. This can be clearly seen from Fig. 1, which displays the band structures of two polarization modes for a triangular lattice of isotropic dielectric cylinders in air. The cylinders have a refractive index of $n = 3.6$ and a filling fraction of $f = 0.4$. Two band gaps open for the E-polarization mode (plotted in solid lines), i.e., the 1-2 band gap and the 3-4 band gap. For the H-polarization mode a band gap is opened between 1-2 bands. However, the H 1-2 band gap lies between the E 1-2 and 3-4 band gaps; thus no absolute band gap is present.

The case can be changed by introducing the anisotropy in the dielectric of cylinders. If we can move upwards the H 1-2 band gap so that it can overlap with the E 3-4 band gap, or if we can shift it downwards as to overlap the E 1-2 band gap, an absolute band gap will be opened. As the photonic band frequency is somewhat inverse with respect to refractive index contrast, this means that we must choose in the former case a refractive index for the H-polarization mode lower than that for the E-polarization mode, namely, $n_e > n_o$, a positive uniaxial crystal. In the latter case, we should select a negative uniaxial material with $n_e < n_o$.

Following this idea, we investigate the dependence of band gap positions on the refractive index for both polarization modes, in order to design photonic crystals with optimal band gaps. As an example, we first consider the triangular lattice of dielectric cylinders in air. The filling fraction of cylinders is fixed as $f = 0.4$. The results are displayed in Fig. 2. A band gap is present for the H-polarization mode at a refractive index larger than 3.0. Two wide band gaps still open for the E-polarization mode at a refractive index as low as $n = 2.0$. However, the band gaps of the two modes do not overlap at all refractive indices. The top edge of the H 1-2 band gap is always lower than the bottom edge of the E 3-4 band gap, while the bottom edge of the H 1-2 band gap is always higher than the top edge of the E 1-2 band gap. Therefore, no absolute band gap is present at all refractive indices.

As conceptualized above, the optimal overlap of E and H band gaps can be obtained by introducing anisotropy in material dielectricity. This is verified when one looks into Fig. 2. The H 1-2 band gap can overlap either with the E 1-2 band gap at a lower refractive index or with the E 3-4 band gap at a higher refractive index. Given an anisotropy sufficient enough, the band gaps will match completely and the largest absolute band gap can be achieved. In particular, consider the large H 1-2 band gap at $n_o = 4.0$, which lies between $0.278-0.333(2\pi c/a)$, where c is the light speed in vacuum and a is the lattice constant of a triangular lattice. Its top edge overlaps with that of the E 3-4 band gap at $n_e = 5.2$, and its bottom edge overlaps with that of the E 3-4 band gap at $n_e = 4.8$. Therefore, the two band gaps wholly overlap each other at the range of $4.8 \leq n_e \leq 5.2$. Similarly, it can be found that this H 1-2 band gap also completely overlaps the E 1-2 band gap at the range of $2.6 \leq n_e \leq 2.8$. The anisotropy to obtain the optimal absolute band gap by a positive crystal is weaker than that by a negative crystal; thus it is easier in experiment to fabricate from positive uniaxial material 2D PBG crystals with optimal band gaps.

Such a concept is also applicable to other lattice types and atom configurations. Figure 3 displays the dependence of band gap positions on the refractive index contrast for both polarization modes in a square lattice of dielectric

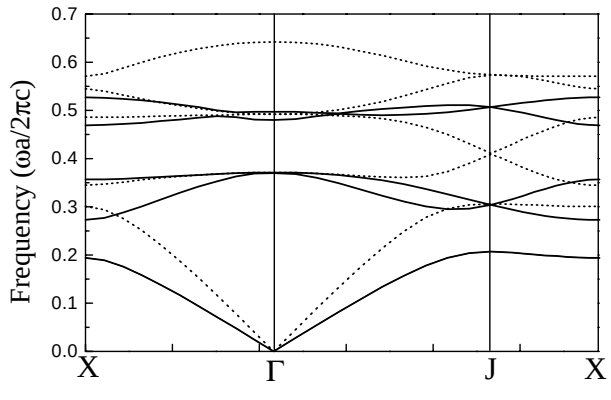

FIG. 1. Calculated photonic band structure for a triangular lattice of isotropic dielectric cylinders in air for E-polarization (solid lines) and H-polarization (dotted lines) modes. The cylinders have a refractive index of $n = 3.6$ and a filling fraction of $f = 0.4$.

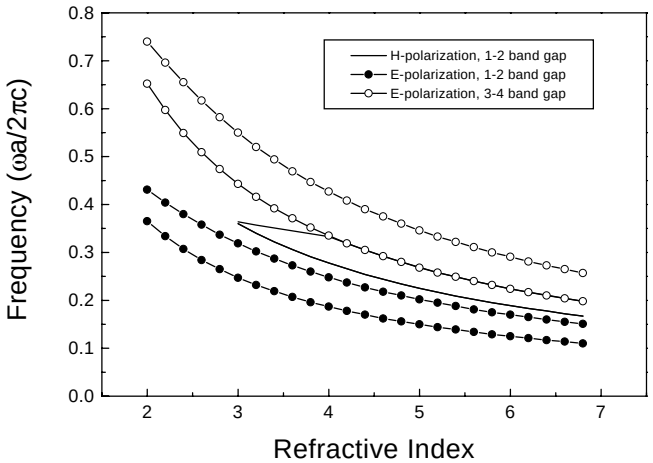

FIG. 2. Dependence of band gap positions on the refractive index for the triangular lattice of dielectric cylinders in air with a filling fraction of $f = 0.4$.

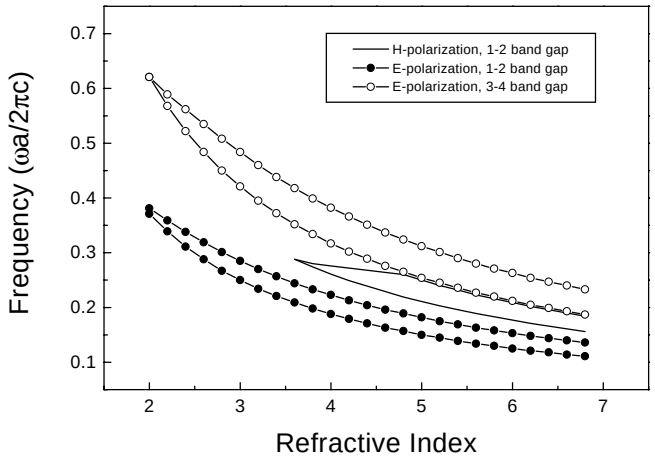

FIG. 3. Dependence of band gap positions on the refractive index for the square lattice of dielectric cylinders in air with a filling fraction of $f = 0.4$.

cylinders in air. The filling fraction of cylinders is fixed as $f = 0.4$. Although the band gap variations are similar to those in triangular lattice, comparing Fig. 3 with Fig. 2, the band gaps are narrower than in triangular lattice. The H 1-2 band gap does not open until at a large refractive index over 3.6 and reaches its maximum size at $n = 4.8$.

According to Fig. 3, no absolute band gap is present in such isotropic photonic crystals at any refractive index. However, an absolute band gap can also be opened by the introduction of sufficient anisotropy into material dielectricity, shifting the H 1-2 band gap either upwards or downwards to overlap with the E 3-4 band gap or the E 1-2 band gap, respectively. Similar to a triangular lattice, an optimal absolute band gap can be obtained by matching the relative position of the H 1-2 band gap either with the E 3-4 band gap or with the E 1-2 band gap, corresponding to the selection of positive crystals or negative crystals. Because of narrower E 1-2 and 3-4 band gaps, the matching condition is more strict than for triangular lattice. For example, the large H 1-2 band gap at $n_o = 4.8$ can completely overlap the E 3-4 band gap at the narrow range of $5.9 \leq n_e \leq 6.0$ and overlap the E 1-2 band gap only at about $n_e = 3.1$. It is also favorable to obtain from positive crystals the optimal absolute band gaps in such square lattice structures.

In principle the optimal absolute band gaps can be obtained for any 2D photonic crystals, as the adjustment of band structures by the anisotropy in dielectricity is so effective. However, in practice, due to limited anisotropic materials [17], such an optimal match in band gaps cannot fully be achieved because it needs very strong anisotropy in material dielectricity. Nevertheless, the anisotropy is still of much help to create and increase absolute band gaps in 2D PBG structures.

As a practical example, we consider 2D PBG structures made from Te (tellurium), which is a kind of positive uniaxial crystal with principal indices of $n_e = 6.2$ and $n_o = 4.8$ in the wavelength regime between 3.5 and 35 μm.

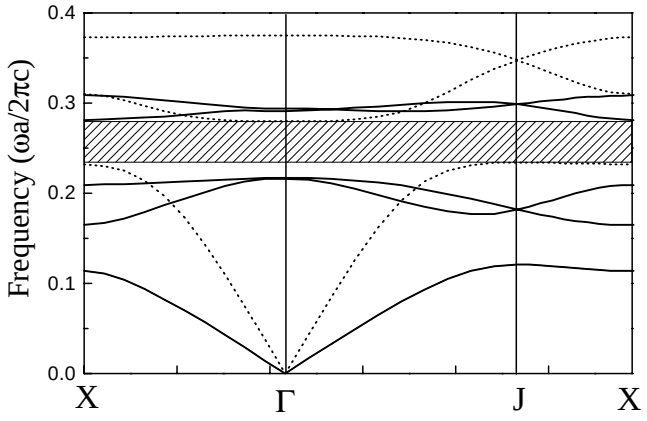

FIG. 4. Calculated photonic band structures of a triangular lattice of Te cylinders in air for E-polarization (solid lines) and H-polarization (dotted lines) modes. The filling fraction of Te cylinders is $f = 0.4$. An absolute band gap (crosshatched region) is present between $0.234-0.280(2\pi c/a)$.

As the free carrier absorption is quite weak for Te in the infrared regime (absorption coefficient $\alpha \simeq 1$ cm^{-1}), the imaginary parts of the complex refractive indices can be neglected compared with their real parts, and the photonic band structures will not be changed. The absorption will not become a serious problem as a photonic crystal consisting of several tens of unit cell layers is thick enough for practical applications.

The photonic band structures for triangular and square lattices of Te cylinders in air are displayed in Figs. 4 and 5, respectively. The filling fractions of cylinders are both $f = 0.4$ and the extraordinary axis of Te is chosen parallel to the extension direction of cylinders. It is evident that an absolute band gap is present in both lattice structures, which results from the overlap of the H 1-2 band gap with the E 3-4 band gap, consistent with the analysis of anisotropy match for band gaps shown in Figs. 2 and 3. The absolute band gap for the triangular lattice has a

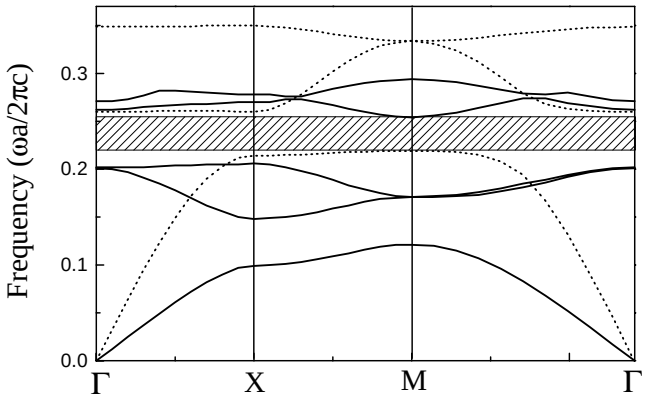

FIG. 5. Calculated photonic band structures of a square lattice of Te cylinders in air for E-polarization (solid lines) and H-polarization (dotted lines) modes. The filling fraction of Te cylinders is $f = 0.4$. An absolute band gap (crosshatched region) lies between $0.219-0.254(2\pi c/a)$.

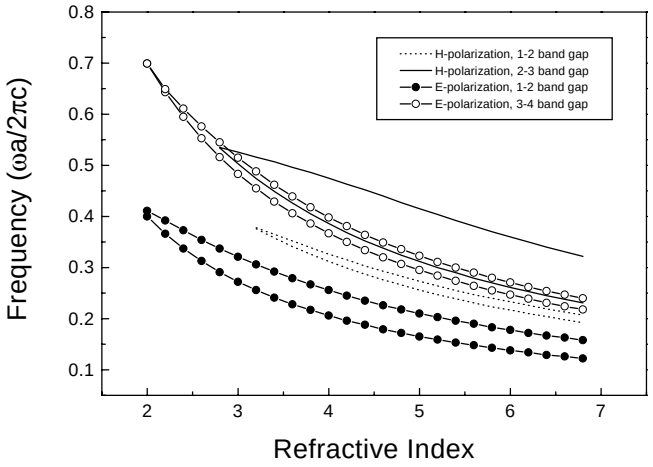

FIG. 6. Dependence of band gap positions on the refractive index for a square lattice of air cylinders in dielectric medium. The cylinders have a filling fraction of $f = 0.7$.

width of $\Delta\omega = 0.046(2\pi c/a)$, and a band gap to midgap ratio of $\Delta\omega/\omega_g = 17.9\%$. For the square lattice we have $\Delta\omega = 0.035(2\pi c/a)$ and $\Delta\omega/\omega_g = 14.8\%$.

As to PBG structures with air cylinders in background dielectric, which exhibit absolute band gaps in both square and triangular lattices [18], the anisotropy in dielectricity can also improve the size of absolute band gap. The principle is essentially the same as in crystals of dielectric cylinders in air.

Figure 6 displays the dependence of band gap positions on the refractive index contrast for both polarization modes in a square lattice of air cylinders embedded in dielectric medium. The filling fraction of air holes is $f = 0.7$. It is evident that the H 2-3 band gap overlaps partially with the E 3-4 band gap at a refractive index of background medium larger than 2.8. Photonic crystals composed of negative material with a weak anisotropy will move upwards the E 3-4 band gap relative to the H 2-3 band gap. This will improve remarkably the two band gaps overlapping and the absolute band gap can be increased 2–3 times. As an example, the absolute band gap for isotropic photonic crystal at $n = 4.0$ has a width of $\Delta\omega = 0.012(2\pi c/a)$. Yet the anisotropic PBG structure with $n_e = 4.0$ and $n_o \geq 4.2$ exhibits an absolute band gap with $\Delta\omega = 0.031(2\pi c/a)$, about 3 times the size of that in isotropic crystals. The E 3-4 and H 2-3 band gaps can be matched optimally by weak negative anisotropy in a wide range of refractive index. Yet it is difficult in practice to match the E 1-2 band gap with the H 2-3 band gap, as this will require very strong anisotropy in negative materials. Simulations made for the triangular lattice of air cylinders in background dielectric demonstrate that large absolute band gaps also open for anisotropic 2D PBG structures.

As a conclusion, we have shown that the anisotropy in material dielectricity for both square and triangular lattices can increase the size of absolute photonic band gap remarkably. As the refractive index for the E-polarization and H-polarization modes can be chosen different, the band gaps can be adjusted and matched to overlap optimally. In particular, the positive uniaxial materials are more favorable in improving the absolute band gap of photonic crystals consisting of dielectric cylinders in air, while for crystals composed of air holes in dielectric medium, negative uniaxial materials are more competent. Because of large varieties of anisotropic materials in Nature, this opens up a new scope for designing the band gap of 2D photonic crystals.

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