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# Modulation of photonic band structures with dielectric anisotropy

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**Abstract.** By the multiple scattering method and the extended Mie theory, we have calculated the photonic band structure of the photonic crystals consisting of the dielectric spheres with uniaxial/biaxial anisotropy. The results demonstrate that for fcc lattice structure there exist two partial photonic band gaps which does not appear in the isotropic case. Among them, the lower one, lying between the second and the third bands, exists in one third of the first Brillouin zone, while the upper one, opening between the fourth and fifth bands, can appear simultaneously in the rest two thirds of the first Brillouin zone. The effects of anisotropy on the band structures are studied as well, which suggests the biaxial anisotropy are much more flexible than the uniaxial anisotropy in modulating the band structures.

**PACS.** 42.70.Qs Photonic bandgap materials – 42.25.Fx Diffraction and scattering – 42.25.-p Wave optics

## 1 Introduction

Since the pioneering work of Yablonovitch and John [1,2], there appears a growing interest in finding the photonic crystals (PCs) with photonic band gaps (PBGs). A PBG means in some frequency range the electromagnetic (EM) waves are prohibited from propagation in certain or all directions, corresponding to partial and complete PBG, respectively. With the existence of PBGs, the spontaneous emission can be controlled in PCs, which results in many potential applications in optical and electronic devices such as selective reflectors, optical polarizers, laser cavities, optical transistors, solar cells and so on [1–7].

Considerable efforts have been devoted to this field, the results suggest that contrast of dielectric constant, the shape of the dielectric structure and the topological connectivity of the dielectric materials play a crucial role in opening the PBGs [6,8]. For the PCs consisting of isotropic dielectric spheres, the complete PBGs can be found in the diamond structure and inverse opal face centered cubic (fcc) structure [9–13]. As for fcc lattice structure and simple cubic (sc) lattice structure consisting of isotropic dielectric spheres, there exist only partial PBG because of the symmetry-induced degeneracy at the $W$ point for fcc and $M$ point for sc in the first Brillouin zone [7,14,15].

Introduction of anisotropy, either in shape or dielectricity can break down the symmetry, leading to the lift of degeneracy, which may result in the appearance of complete PBGs [15–27]. The PCs composed of nonspherical dielectric atoms were revealed to exhibit complete PBGs [17–21]. Similar to the introduction of the asymmetry in atomic configuration, the introduction of anisotropy in dielectricity should achieve the same purpose. The studies on two dimensional PCs show that anisotropy in dielectricity is effective in opening up complete PGBs [22–24]. Studies on three dimensional case have also been performed [15,25–27], one of which suggests that for PCs consisting of uniaxially birefringent dielectric spheres, a partial PBG is found in one third of the first Brillouin zone for fcc, sc and body center cubic (bcc) lattice structures [15].

In present work, besides uniaxial anisotropy, we introduce biaxial anisotropy as well in dielectricity which renders us much more flexibility in modulating the band structures. Not only the partial PBG in one third of the first Brillouin zone is found, another partial PBG in the rest two thirds of the first Brillouin zone is found simultaneously for fcc lattice structure. With the adjustment of the anisotropy the band structure can be optimized, leading to the appearance of the appropriate PBGs.

In calculating photonic band structures, the most frequently adopted technique is the plane-wave expansion method, which can offer reliable results in most cases. Nevertheless, if there exists the sharp change of the EM waves at the interface or the anisotropy of the dielectricity, it will suffer from the difficulty of bad convergence [12,28]. In our calculation multiple scattering method, named also as KKR method [29,30], is employed. Compared with plane-wave expansion method, it bears the advantage of numerical accuracy in addition to computer time saving in

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calculating the spherical scattering problem, since it takes into account the boundary conditions at the interface properly. The key task in applying the KKR method is to obtain the scattering matrix of single dielectric sphere. For isotropic dielectric sphere, the scattering matrix is easily obtained within the Mie theory [31]. However, for dielectric sphere with anisotropy, to obtain the scattering matrix is a nontrivial job. Fortunately, the scattering matrices of uniaxially and biaxially dielectric sphere have been obtained exactly within the extended Mie theory in our previous work [27,32].

After incorporating the scattering matrix into the KKR method, the band structure can be calculated. We have written computer code to implement KKR method in calculating the band structure of 3D PCs consisting of uniaxially/biaxially dielectric spheres. The program works efficiently and offers reliable results. In our calculation the maximal angular momentum is taken as $n_c = 7$, which guarantees a good convergence of solution.

## 2 Band structures of PCs with uniaxial/biaxial anisotropy

For the anisotropic materials, the dielectric constant are dyadic (second rank tensor). Herein, dielectric constant with biaxial anisotropy can be written as

$$\epsilon_s \widehat{\epsilon} = \epsilon_s \begin{pmatrix} \epsilon_1 & 0 & 0 \\ 0 & \epsilon_2 & 0 \\ 0 & 0 & \epsilon_3 \end{pmatrix}, \tag{1}$$

where, without loss of generality, we take principal axis $\epsilon_3$ as extraordinary axis and normalize it to unit, the other two principal axes $\epsilon_1$ and $\epsilon_2$ are taken as 2 ordinary axes. Uniaxial anisotropy, corresponding to $\epsilon_1 = \epsilon_2$, can be considered as a special case of biaxial anisotropy. For the convenience of later discussion, the permittivity tensor of the dielectric sphere with uniaxial anisotropy is written in the form

$$\epsilon_s \widehat{\epsilon} = \epsilon_s \begin{pmatrix} 1 - \delta\epsilon_{||} & 0 & 0 \\ 0 & 1 - \delta\epsilon_{||} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{2}$$

where $\delta\epsilon_{||}$ is a positive number with $\delta\epsilon_{||} < 1$ in our later discussion. The parameter $\delta\epsilon_{||}$ can be used to evaluate the anisotropy, i.e. the larger it is, the stronger the anisotropy is to be. As for the isotropic case, it corresponds to $\delta\epsilon_{||} = 0$ or $\epsilon_1 = \epsilon_2 = \epsilon_3$. Herein the permeability $\mu = 1.0$ for nonmagnetic material.

In the calculations of the band structures, we take $\epsilon_s = 35$, while $\epsilon_1$, $\epsilon_2$ can be modulated to find appropriate values (for uniaxial case, $\delta\epsilon_{||}$ is modulated). The extraordinary principal axis $\epsilon_3$ is oriented along [001] direction and the two ordinary axes $\epsilon_1$ and $\epsilon_2$ are along [100] and [010] directions respectively in fcc lattice structure. In calculating the band structures of PCs consisting of isotropic dielectric spheres, only 1/48 of the first Brillouin zone need to be considered due to the symmetry. However, herein with the existence of anisotropy most of the symmetries break down, the only one kept is the inverse symmetry which means that the points $(a, b, c)$ and $(-a, -b, -c)$ are equivalent. To that extent, the calculation of the band structure should be performed over one half of the whole first Brillouin zone for PC composed of general biaxial anisotropic dielectric spheres, namely, one has to compute for twenty-four 1/48 of the first Brillouin zone.

Different from the isotropic case, the anisotropy (either uniaxial or biaxial) introduced herein breaks down the symmetry to some extent, which results in the lift of degeneracy. As a result band structure will split, then we can expect the appearance of new PBGs or the close of original PBGs. We have shown in Figures 1 the band structures of PCs consisting of uniaxial dielectric spheres with $\epsilon_s = 35.0$, $\epsilon_3 = 1.0$, the filling ratio $f = 0.25$, while $\delta\epsilon_{||} = 0.65$, 0.60, 0.55, 0.50 and 0.45 for Figures 1a–e, respectively. Figure 1f corresponds to the band structure of PC consisting of isotropic dielectric spheres with filling fraction $f = 0.25$, the same as that of the anisotropic case, and $\epsilon = 15.0$, which locates in between the minimum and maximum values of $\epsilon_s(1 - \delta\epsilon_{||})$ in Figure 1, for the convenience of comparison. The high symmetry points in the band structures are $\Gamma = (0, 0, 0)$, $X = \frac{2\pi}{a}(0, 1, 0)$, $U = \frac{2\pi}{a}(\frac{1}{4}, 1, \frac{1}{4})$, $L = \frac{2\pi}{a}(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, $W = \frac{2\pi}{a}(0, 1, \frac{1}{2})$, $K = \frac{2\pi}{a}(0, \frac{3}{4}, \frac{3}{4})$. It is evident that between the fourth and the fifth bands in Figures 1b–d there exist partial PBGs, which results from the anisotropy-induced band splitting at $\Gamma$ point for 4–5 band in isotropic case shown in Figure 1f. Through modulating the values of $\delta\epsilon_{||}$, we can obtain the band structure with the largest partial PBG which is shown in Figure 1c for $\delta\epsilon_{||} = 0.55$. Consequently, to obtain the maximum PBG taking appropriate dielectric anisotropy is very important. With the decrease of $\delta\epsilon_{||}$ the band splitting for 3–4 photonic bands becomes prominent, leading to the overlap of the fourth and the fifth photonic bands with each other, as shown in Figure 1e, when $\delta\epsilon_{||}$ is less than 0.45, the PBG closes eventually due to this overlap. On the contrary if $\delta\epsilon_{||}$ increases the band splitting for 1–2 photonic bands becomes prominent, so that the second and the fifth photonic bands overlap with each other, as shown in Figure 1a, resulting in the close of the PBG when $\delta\epsilon_{||} > 0.7$. Notice that the band structure shown in Figure 1 is just for one 1/48 of the first Brillouin zone. We have also calculated the photonic band structures in other partial Brillouin zones with the same parameters. Our results shows that the partial PBG exists in other 31 partial (1/48) Brillouin zones as well. It is therefore concluded that the PBG between the forth and fifth bands can be found in $32 \times 1/48 = 2/3$ of the first Brillouin zone.

Besides the partial PBG in Figure 1 appearing between the forth and fifth bands, there exists another partial PBG for PCs consisting of uniaxial dielectric spheres in other partial regions of the first Brillouin zone. The band structures are shown in Figure 2. The dielectric parameters are $\epsilon_s = 35.0$, $\epsilon_3 = 1.0$, the filling ratio $f = 0.25$, while $\delta\epsilon_{||} = 0.75$, 0.65, 0.35 and 0.15 for Figures 2a–d, respectively. The symmetry points in the band

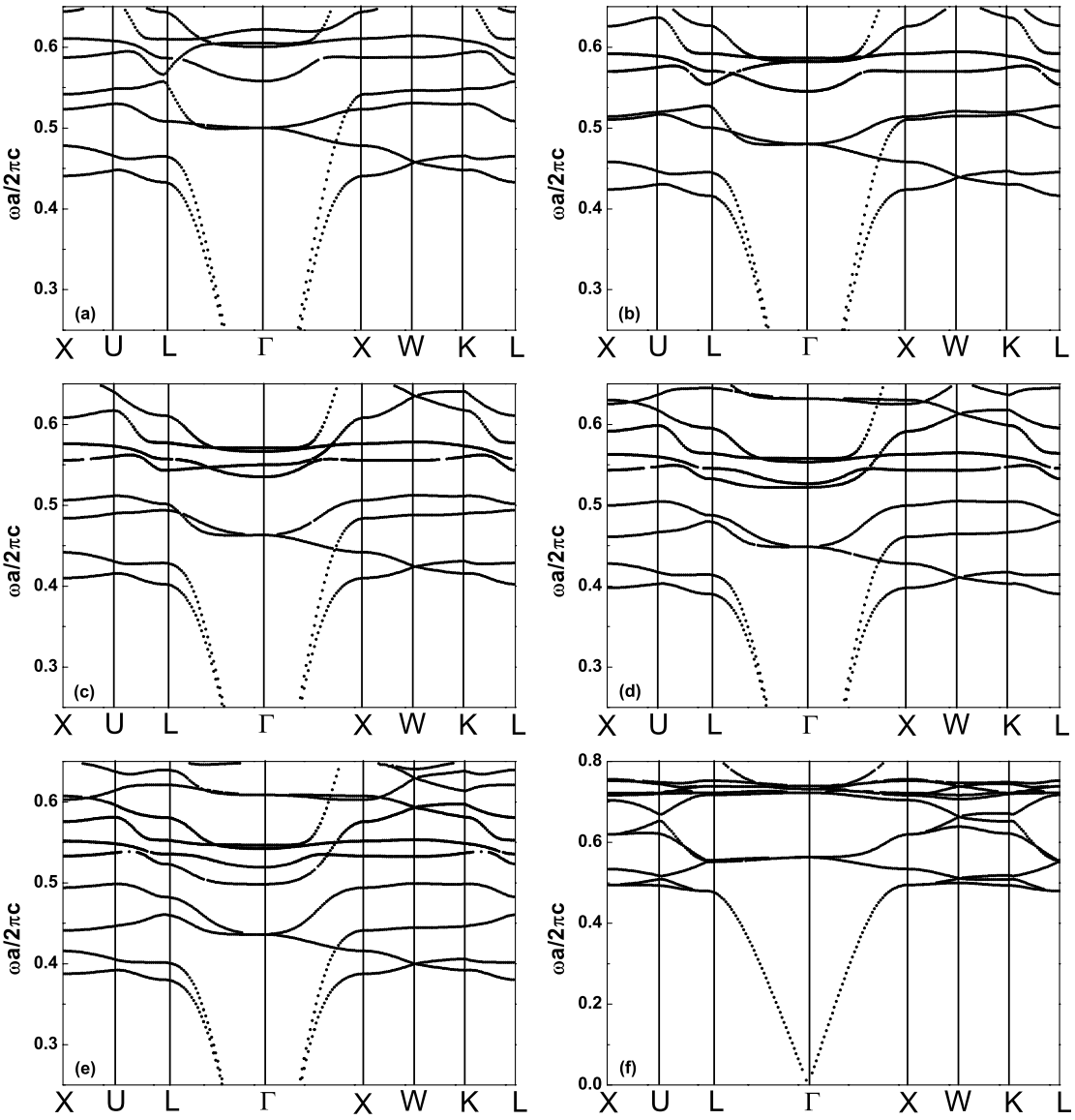


**Fig. 1.** Calculated photonic band structures of a PC consisting of uniaxial dielectric spheres in fcc lattice with high symmetry points in the first Brillouin zone given by $\Gamma = (0,0,0)$, $X = \frac{2\pi}{a}(0,1,0)$, $U = \frac{2\pi}{a}(\frac{1}{4},1,\frac{1}{4})$, $L = \frac{2\pi}{a}(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, $W = \frac{2\pi}{a}(0,1,\frac{1}{2})$, $K = \frac{2\pi}{a}(0,\frac{3}{4},\frac{3}{4})$. The filling fraction is $f = 0.25$. The extraordinary axis, corresponding to the principal axis $\epsilon_3$ with $\epsilon_3 = 1.0$, is oriented along [001] direction and the 2 ordinary axes $\epsilon_1$ and $\epsilon_2$ are along [100] and [010] directions respectively with their values decided by (a) $\delta\epsilon_{||} = 0.65$; (b) $\delta\epsilon_{||} = 0.60$; (c) $\delta\epsilon_{||}$=0.55; (d) $\delta\epsilon_{||} = 0.50$; (e) $\delta\epsilon_{||} = 0.45$; (f) corresponding to the PC composed of isotropic dielectric spheres with $\epsilon = 15.0$ and filling fraction $f = 0.25$.

structures are $\Gamma = (0,0,0)$, $X = \frac{2\pi}{a}(0,0,1)$, $U = \frac{2\pi}{a}(\frac{1}{4},\frac{1}{4},1)$, $L = \frac{2\pi}{a}(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, $W = \frac{2\pi}{a}(0,\frac{1}{2},1)$, $K = \frac{2\pi}{a}(0,\frac{3}{4},\frac{3}{4})$. Notice that the symmetric points in the Brillouin zone for Figure 2 are different from those in Figure 1. It can be seen from the band structures that the degeneracy at $W$ point for 2–3 photonic band, shown in Figure 1f, has been canceled by the anisotropy, which results in the formation of the PBG. The PBG exists in a wide range of $\delta\epsilon_{||}$ (from $\delta\epsilon_{||} = 0.15$ to $\delta\epsilon_{||} = 0.75$), therefore it is a robust one for uniaxial case. If $\delta\epsilon_{||}$ is greater than 0.75, the splitting for 1–2 and 3–4 becomes large so that the second and the third bands overlap with each other, as shown in Figure 2a, which leads to the close of the PBG. On the contrary if $\delta\epsilon_{||}$ are less than 0.15 the splitting between the fifth and the sixth bands becomes prominent so that the fifth band overlap with the second band, shown in Figure 2d, which gives rise to the close of the PBG. In addition, another partial PBG can be found between 8–9 bands, shown in Figure 2c, which is consistent with Li [15]. But in Li's work the PBG in Figure 1 is not found, the reason lies in that the anisotropy is not large enough [$\delta\epsilon_{||}$ should be greater than 0.45, while in their work $\epsilon_s = 38.44$, $\delta\epsilon_{||} = 0.401$, $\epsilon_3 = 1.0$ (the parameters from Tellurium)]. The partial PBG between 8–9 bands is much weaker than that between 2–3 bands in that a small change of the filling ratio or anisotropy will result in the close of it. Compared

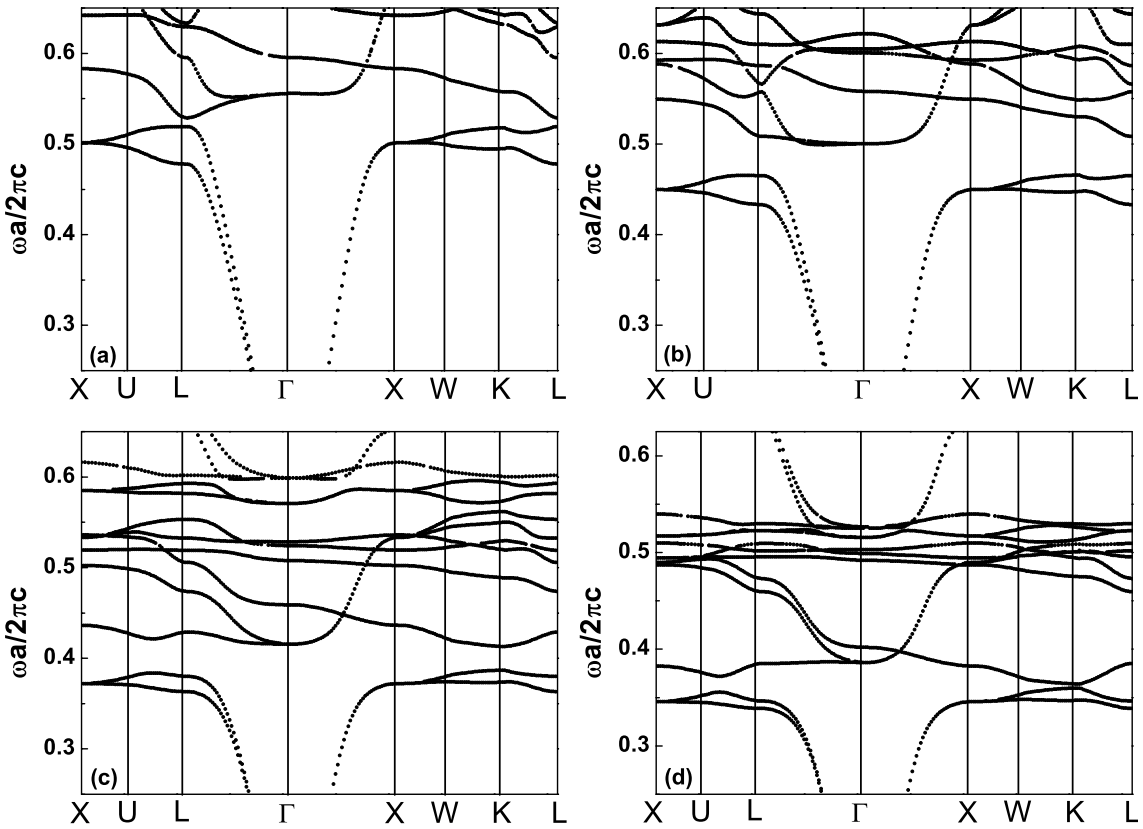


**Fig. 2.** Calculated photonic band structures of a PC consisting of uniaxial dielectric spheres in fcc lattice with high symmetry points in the first Brillouin zone given by $\Gamma = (0,0,0)$, $X = \frac{2\pi}{a}(0,0,1)$, $U = \frac{2\pi}{a}(\frac{1}{4},\frac{1}{4},1)$, $L = \frac{2\pi}{a}(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, $W = \frac{2\pi}{a}(0,\frac{1}{2},1)$, $K = \frac{2\pi}{a}(0,\frac{3}{4},\frac{3}{4})$. The filling fraction is $f = 0.25$. The extraordinary axis, corresponding to the principal axis $\epsilon_3$ with $\epsilon_3 = 1.0$, is oriented along [001] direction and the 2 ordinary axes $\epsilon_1$ and $\epsilon_2$ are along [100] and [010] directions respectively with their values decided by (a) $\delta\epsilon_{||} = 0.75$; (b) $\delta\epsilon_{||} = 0.65$; (c) $\delta\epsilon_{||} = 0.35$; (d) $\delta\epsilon_{||} = 0.15$.

with the upper lying PGB in Figure 1, the lower lying PBG in Figure 2 prefers small anisotropy, which can be reflected in that it persistingly exists even when $\delta\epsilon_{||}$ is nearly equal to zero (corresponding to the isotropic case).

Now we turn to the case in which the PCs consist of the dielectric spheres with biaxial anisotropy. Similar to the uniaxial case, there still exist two partial PBGs, which are due to the lift of degeneracy in band structure. The analysis can be performed similarly to the uniaxial case. The upper PBG, lying between the forth and fifth bands seems very stable against the biaxial anisotropy. For instance, when $\epsilon_s = 35.0$, $\epsilon_1 = 0.4$ and $\epsilon_3 = 1.0$ with the filling ratio $f = 0.25$, the PBG persists for $\epsilon_2$ varying from 0.35 to 0.95. In addition, the width of the PBG reaches its maximum at $\epsilon_2 = 0.50$, indicating that the introduction of biaxial anisotropy can further enlarge the PBG between forth and fifth bands, implying more flexibility in modulating the band structure. The lower PBG opening between the second and the third bands, on the other hand, appears not as stable as the upper one against the introduction of biaxial anisotropy. For example, for the case with $\epsilon_s = 35.0$, $\epsilon_1 = 0.4$, $\epsilon_3 = 1.0$, and $f = 0.25$, the PBG exists for $0.30 < \epsilon_2 < 0.55$, with its maximum width occurring at $\epsilon_2 = 0.4$ (corresponding to uniaxial case with $\delta\epsilon_{||} = 0.60$), which implies that the introduction of the biaxial anisotropy is unfavorable to the lower PBG. In addition, while larger anisotropy seems to favorable to the upper PBG lying between the forth and the fifth bands, the lower PBG between second and the third bands prefers smaller anisotropy.

Finally, we present in Figure 3 the band structures of PCs consisting of biaxial dielectric spheres in six neighboring partial Brillouin zones, where $\epsilon_s = 35.0$, $\epsilon_1 = 0.40$, $\epsilon_2 = 0.45$, $\epsilon_3 = 1.0$, the filling fraction $f = 0.25$. The high symmetry points are (a) $\Gamma = (0,0,0)$, $X = \frac{2\pi}{a}(0,0,1)$, $U = \frac{2\pi}{a}(\frac{1}{4},\frac{1}{4},1)$, $L = \frac{2\pi}{a}(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, $W = \frac{2\pi}{a}(0,\frac{1}{2},1)$, $K = \frac{2\pi}{a}(0,\frac{3}{4},\frac{3}{4})$; (b) the same as (a) except $W = \frac{2\pi}{a}(\frac{1}{2},0,1)$, $K = \frac{2\pi}{a}(\frac{3}{4},0,\frac{3}{4})$; (c) $\Gamma = (0,0,0)$, $X = \frac{2\pi}{a}(0,0,-1)$, $U = \frac{2\pi}{a}(\frac{1}{4},\frac{1}{4},-1)$, $L = \frac{2\pi}{a}(\frac{1}{2},\frac{1}{2},-\frac{1}{2})$, $W = \frac{2\pi}{a}(0,\frac{1}{2},-1)$, $K = \frac{2\pi}{a}(0,\frac{3}{4},-\frac{3}{4})$; (d) the same as (c) except $W = \frac{2\pi}{a}(\frac{1}{2},0,-1)$, $K = \frac{2\pi}{a}(\frac{3}{4},0,-\frac{3}{4})$; (e) $\Gamma = (0,0,0)$, $X = \frac{2\pi}{a}(1,0,0)$, $U = \frac{2\pi}{a}(1,\frac{1}{4},-\frac{1}{4})$, $L = \frac{2\pi}{a}(\frac{1}{2},\frac{1}{2},-\frac{1}{2})$, $W = \frac{2\pi}{a}(1,0,-\frac{1}{2})$, $K = \frac{2\pi}{a}(\frac{3}{4},0,-\frac{3}{4})$; (f) the same as (e) except $W = \frac{2\pi}{a}(1,\frac{1}{2},0)$, $K = \frac{2\pi}{a}(\frac{3}{4},\frac{3}{4},0)$. It can be seen from the diagram that a partial PBG (the lower one) lying between the second and the third bands exists in Figures 3a and b and another partial PBG (the upper one) lying between the fourth and the fifth bands exists in Figures 3c–f. In the next six neighboring partial Brillouin zone the partial

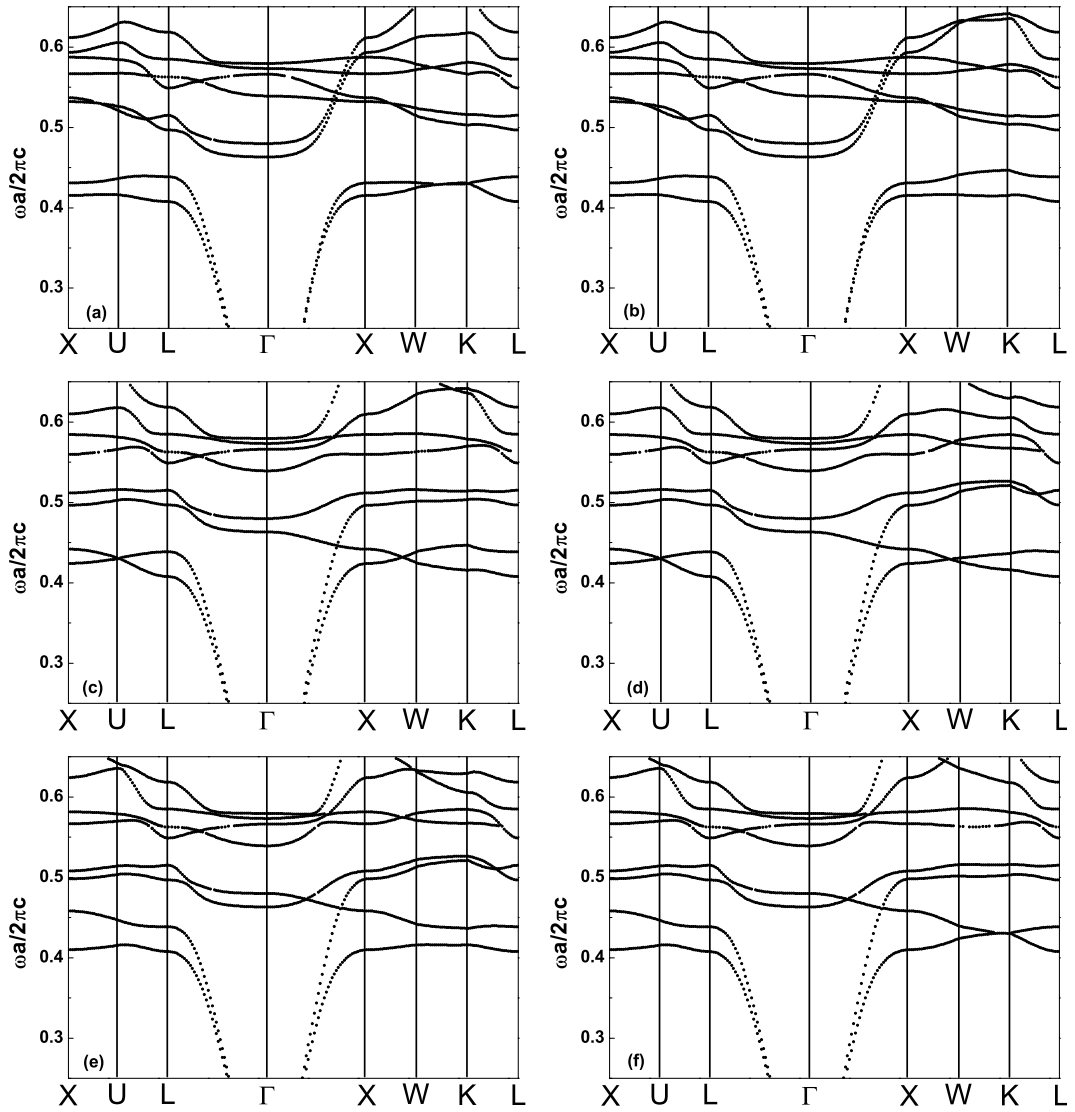


**Fig. 3.** Calculated photonic band structures of a PC consisting of biaxial dielectric spheres in fcc lattice with high symmetry points in the first Brillouin zone given by (a) $\Gamma = (0,0,0)$, $X = \frac{2\pi}{a}(0,0,1)$, $U = \frac{2\pi}{a}(\frac{1}{4},\frac{1}{4},1)$, $L = \frac{2\pi}{a}(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, $W = \frac{2\pi}{a}(0,\frac{1}{2},1)$, $K = \frac{2\pi}{a}(0,\frac{3}{4},\frac{3}{4})$; (b) the same as (a) except $W = \frac{2\pi}{a}(\frac{1}{2},0,1)$, $K = \frac{2\pi}{a}(\frac{3}{4},0,\frac{3}{4})$; (c) $\Gamma = (0,0,0)$, $X = \frac{2\pi}{a}(0,0,-1)$, $U = \frac{2\pi}{a}(\frac{1}{4},\frac{1}{4},-1)$, $L = \frac{2\pi}{a}(\frac{1}{2},\frac{1}{2},-\frac{1}{2})$, $W = \frac{2\pi}{a}(0,\frac{1}{2},-1)$, $K = \frac{2\pi}{a}(0,\frac{3}{4},-\frac{3}{4})$; (d) the same as (c) except $W = \frac{2\pi}{a}(\frac{1}{2},0,-1)$, $K = \frac{2\pi}{a}(\frac{3}{4},0,-\frac{3}{4})$; (e) $\Gamma = (0,0,0)$, $X = \frac{2\pi}{a}(1,0,0)$, $U = \frac{2\pi}{a}(1,\frac{1}{4},-\frac{1}{4})$, $L = \frac{2\pi}{a}(\frac{1}{2},\frac{1}{2},-\frac{1}{2})$, $W = \frac{2\pi}{a}(1,0,-\frac{1}{2})$, $K = \frac{2\pi}{a}(\frac{3}{4},0,-\frac{3}{4})$; (f) the same as (e) except $W = \frac{2\pi}{a}(1,\frac{1}{2},0)$, $K = \frac{2\pi}{a}(\frac{3}{4},\frac{3}{4},0)$. The filling fraction is $f = 0.25$. The extraordinary axis, corresponding to the principal axis $\epsilon_3$ with $\epsilon_3 = 1.0$, is oriented along [001] direction and the ordinary axis $\epsilon_1$ is along [100] direction with the value $\epsilon_1 = 0.40$, the ordinary axis $\epsilon_2$ is along [010] direction with the value $\epsilon_2 = 0.45$.

PBGs appear in the same sequence. Therefore, it is concluded that the lower partial PBG appears in one third of the first Brillouin zone, while the upper one exists, simultaneously, in the rest two thirds of the first Brillouin zone, namely, the two partial PBGs appear alternatively, or, complementarily, in the first Brillouin zone. One physical implication of this property is that while light of certain frequency is prohibited in certain direction, the electromagnetic wave of some other frequency can't propagate in some other directions. By rotating the PC sample, one is expected to control the passing frequency of the electromagnetic radiation, giving rise to an alternative potential handle for the manipulation of light.

## 3 Summary and conclusions

We have investigated the photonic band structures of the fcc lattice composed of dielectric spheres with uniaxial or biaxial anisotropy in the background of air. By incorporating the scattering matrix into the KKR method, the photonic band structures are calculated efficiently. Anisotropy-induced splitting of band structure leads to the lift of degeneracy existing in isotropic case, which results in the appearance of the PBG. For PCs consisting of uniaxial/biaxial dielectric spheres we have found two partial PBGs among which the lower one lies between the second and the third bands and the upper one lies between

the fourth and the fifth bands. The lower PBG exists in one third of the first Brillouin zone while the upper one can appear, simultaneously and complementarily, in the rest two third of the first Brillouin zone, suggesting an alternative way for the fabrication of multi-channel selective reflectors. Another potential application of such kind of PC is the capability in controlling light emission, namely if a light source is placed inside the PC, light of some frequency range can only come out from certain direction, while light of other frequency range comes out from some other directions. In addition, our calculation results suggest that the lower one prefer smaller anisotropy and the upper one prefer larger anisotropy. With the variation of the anisotropy, the photonic band structures are modulated, the evolution of the PBGs in different situations are discussed. Compared with uniaxial case, biaxial anisotropy can offer much more flexibility in modulating band structures, which leads to the appearance of desired PBG.

Finally, we note that it may not be easy to realize such systems with extraordinary axis of all constituent spheres aligned in a particular direction. It is, however, believed that applying an external electric field during the fabrication process may be helpful for spherical particles, at least for the case of uniaxial sphere with strong positive uniaxial anisotropy, in aligning their extraordinary axis along nearly uniform direction. The effectiveness of the external electric field lies in that the free energy of the system $F = -\sum_i \mathbf{p}_i \cdot \mathbf{E}_i$ is lowest for the configuration with highest refractive index axis along the direction of the external field since in such a situation $\mathbf{p}_i$ will reach its maximum magnitude. Herein, $\mathbf{p}_i$ is the electric dipole of a sphere and $\mathbf{E}_i$ is the local electric field. In our work, the highest refractive index direction is the direction of the extraordinary axis of dielectric sphere. The relevant details can be found in reference [15].

Another interesting topic is to study the more realistic cases with anisotropy orienting randomly. This kind of structure certainly do not support photonic band structure due to the non-periodicity. Calculation of (local) density of states may be one suitable way to retrieving property information of these structures. We are working along this line by developing a code for local density of states calculation.

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