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LETTER TO THE EDITOR

Opening up complete photonic bandgaps by tuning the orientation of birefringent dielectric spheres in three-dimensional photonic crystals

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Abstract
By using a multiple-scattering method, we study theoretically the photonic band structures of three-dimensional (3D) photonic crystals consisting of birefringent dielectric spheres. Our results demonstrate the possibility of opening up complete photonic bandgaps in 3D simple lattice photonic systems by changing the orientation of the extraordinary axis of the birefringent spheres.

Photonic crystals (PCs) are composite structures with a spatially periodic variation of refractive index [1–4]. Light propagation in PCs can be strongly modulated not only by the introduced periodicity via multiple Bragg scattering but also by the presence of resonant modes of the building components and is then characterized by complicated photonic band structures. If there exist complete photonic bandgaps (PBGs) between photonic bands, the light propagation will be absolutely forbidden and the spontaneous emission is prohibited within the frequency range of the PBG, giving rise to unprecedented degrees of freedom in the manipulation and control of spontaneous emission as well as light propagation, and, therefore, leading to many potential applications in photonics [3, 4], such as frequency selective reflectors, band filters, and low threshold micro-cavity lasers [5, 6].

Great efforts have been made in the search for PCs with complete PBGs, the existence of which is generally determined by many factors, including the contrast of the dielectric constant of the constituents and the geometry of the constituents, as well as the topological connectivity of the constituents [3]. While most PCs studied are composed of isotropic constituents, PCs consisting of anisotropic constituents have recently received some attention, owing to their interesting physical properties [7–15]. The introduction of anisotropy, either in shape or in dielectricity, is expected to render an additional degree of freedom to create the PBGs in PCs through altering the symmetry and thus lifting the degeneracy of the photonic band structures. In particular, the dielectric anisotropy also introduces some degree of tunability of the photonic band structure [16], in addition to the possibility of opening up and improving the complete PBGs. Although in two dimensions it was reported that both shape anisotropy and dielectric anisotropy prove powerful in opening up and improving the complete PBGs [10–12], for three-dimensional (3D) cases a rather pessimistic conclusion was drawn regarding the efficacy of opening PBG in the 3D PCs consisting of a birefringent dielectric constituent in an air background [7–10]. No complete PBGs were found for PCs in simple lattices, such as face-centred cubic (fcc) and simple cubic (sc) lattices, composed of birefringent dielectric spheres in air [8–10]. For dielectric constituents, except the diamond structure, the complete PBGs in 3D simple lattices made of spherical scatterers were found only in the inverse opal fcc structures, where the introduction of anisotropy provides a unique tuning effect through narrowing and closing the PBG that is already present in the inverse opal fcc structures [16].

In this letter, we report a possibility of opening up complete PBGs in 3D PCs with simple lattices through tuning the orientation of the extraordinary axis of the constituent birefringent dielectric spheres. The calculation of the photonic band structures was made based on a multiple-scattering method [17–22]. It is found that in 3D PCs consisting of birefringent dielectric spheres in the fcc and sc lattices a complete PBG may be created by changing the orientation of the extraordinary axis of the birefringent spheres, which in turn suggests a potential approach to obtain some degree of tunability of the photonic band structures. In contrast with liquid crystals in the inverse opal fcc structure [16], the tuning effect here is achieved by opening up a new complete PBG that is forbidden in the isotropic system, instead of narrowing or closing a PBG which is already existent in the isotropic system.

For uniaxially birefringent material, the electric permittivity is a second-rank tensor

$$\overleftrightarrow{\varepsilon} = \varepsilon_s \begin{pmatrix} \varepsilon_r & 0 & 0 \\ 0 & \varepsilon_r & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{1}$$

where $\varepsilon_s\varepsilon_r = n_o^2$ and $\varepsilon_s = n_e^2$, with n_o and n_e denoting the refractive indices in the ordinary and the extraordinary directions. For $\varepsilon_r < 1$ ($\varepsilon_r > 1$), the material is positive (negative) uniaxial. To illustrate our idea, the constituent material of the birefringent dielectric spheres is chosen to be tellurium (Te), which is a positive birefringent crystal with $n_o = 4.8$ and $n_e = 6.2$. However, the basic concept is not limited to the particular material, provided that the principal refractive indices and material birefringence are large enough. PCs considered consist of uniaxially birefringent dielectric spheres, which are arranged in the fcc and sc lattices in an air background. The cubic lattice constant of the fcc and sc lattices is denoted by a and the radius of spheres by r. For the fcc and sc lattices, the filling fraction of dielectric spheres is then given by $f = \frac{16\pi r^3}{3a^3}$ and $\frac{4\pi r^3}{3a^3}$, respectively.

Most photonic band structure calculations have been done by either the plane-wave expansion method (see, e.g., [23]), since it is straightforward and easy to employ, or the finite difference time domain method (see, e.g. [24]), which is widely implemented in the engineering community. These methods have been very successful in dealing with simple dielectric PCs. However, for metallic systems or systems with a rapid spatial variation of refractive index, it is rather difficult to achieve a reliable convergence of the solutions. In particular, sometimes the plane wave expansion method may produce unreliable results [25]. For PCs consisting of non-overlap spheres, the multiple scattering method proves to be most powerful. Since it takes into account the proper boundary conditions of the interface exactly and works on the frequency domain, the multiple-scattering method offers much higher numerical accuracy and needs less computer time in dealing with metallic systems, systems with a rapid spatial variation of the refractive index, or systems consisting of dispersive materials. The central idea of the multiple-scattering method is that the whole system considered is treated as an assembly of scatterers and its scattering properties are taken as sums over individual scatterers. Once the scattering properties of the individual scatterer are characterized by the scattering matrix (or

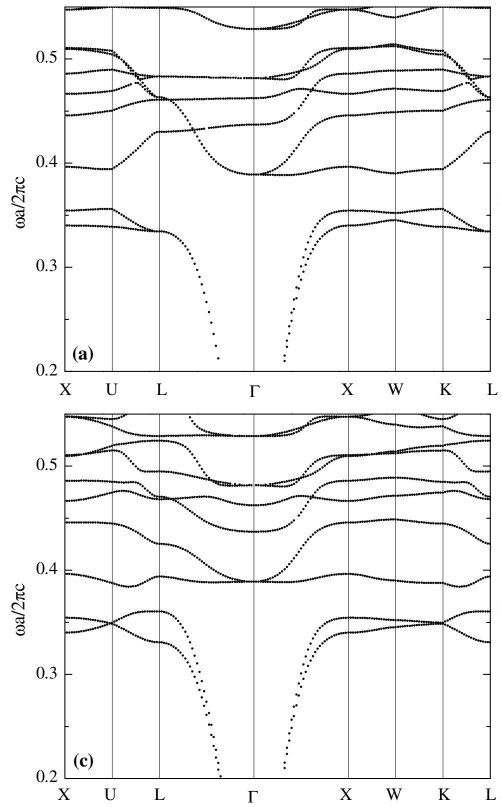

Figure 1. Calculated photonic band structures of a PC consisting of Te spheres in the fcc lattice. The extraordinary axis of Te spheres is oriented along the [111] direction. The filling fraction of Te spheres is $f = 0.3$. The photonic band structures of this PC in the whole Brillouin zone are plotted, equivalently, as a combination of four partial photonic band structures in a fixed partial region of the Brillouin zone (the standard irreducible Brillouin zone of the fcc lattice) with the extraordinary axis of Te spheres oriented along (a) [111], (b) $[\bar{1}11]$, (c) $[1\bar{1}1]$, and (d) $[11\bar{1}]$ directions. The high symmetry points in the irreducible Brillouin zone of the fcc lattice are denoted by $\Gamma = (0,0,0)$, $\mathrm{X} = (2\pi/a)(1,0,0)$, $\mathrm{W} = (2\pi/a)(1,\frac{1}{2},0)$, $\mathrm{K} = (2\pi/a)(\frac{3}{4},\frac{3}{4},0)$, $\mathrm{L} = (2\pi/a)(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, and $\mathrm{U} = (2\pi/a)(1,\frac{1}{4},\frac{1}{4})$.

scattering coefficients for an isotropic sphere), the scattering properties of the entire system can be constructed and the band structure of the PCs can be obtained from the stationary-state solution of the systems. We have developed a general formulation for evaluating the scattering matrix of a sphere with gyrotropic anisotropy [26], of which the uniaxially birefringent sphere is a special case. Here in our photonic band structure calculations, we adopt the multiple-scattering method incorporated with the exact calculation of the scattering matrix for the birefringent sphere. In our calculations, we choose the maximal angular momentum $l_{\max} = 7$, which guarantees a very good convergence of the solutions.

It is well known that the existence of complete PBGs is limited to the diamond structure and the inverse opal fcc structure [23, 25, 27] if the constituent dielectric spheres are isotropic. Partial PBGs can be created in a simple lattice of birefringent Te spheres in an air background [8] when the extraordinary axis of the birefringent spheres is aligned with the [100] direction. No complete PBG is found in the whole Brillouin zone. To show the possibility of opening up a complete PBG in a simple lattice by tuning the orientation of the constituent birefringent

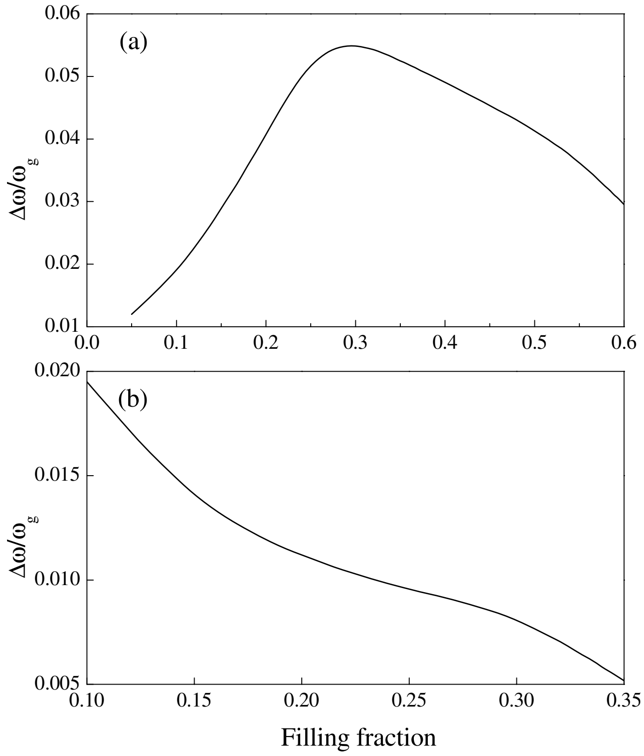

Figure 2. The gap to midgap ratio of (a) the first and (b) second PBGs as a function of the filling fraction for the PC consisting of Te spheres in the fcc lattice. The extraordinary axis of Te spheres is oriented along the [111] direction.

spheres, we reorient the extraordinary axis of the Te spheres along the [111] direction of the fcc lattice. Unlike a PC consisting of isotropic dielectric spheres arranged in the fcc lattice, where the band structure can usually be shown only in 1/48 of the first Brillouin zone, for a PC consisting of anisotropic material, since its symmetry is reduced, in general, we have to do the band calculations in the whole Brillouin zone. In the present work, instead of doing so, we do the calculations in a fixed partial Brillouin zone (the standard irreducible Brillouin zone of the fcc lattice, see e.g., [28], with the coordinates of the high symmetry points of this partial Brillouin zone given in the figure captions). By transforming the electric permittivity dyadic $\overleftrightarrow{\varepsilon}$, we can get the photonic band structures in the whole Brillouin zone. To be specific, in the case of a PC consisting of birefringent spheres with the extraordinary axis oriented along the [111] direction and arranged in the fcc lattice, the photonic band structures in the whole Brillouin zone can be transformed equivalently into the photonic band structures in a fixed partial region of the standard Brillouin zone but with the extraordinary axis of Te spheres along the [111], $[\bar{1}11]$, $[1\bar{1}1]$, and $[11\bar{1}]$ directions.

The calculated photonic band structures for an fcc lattice of Te spheres in air with filling fraction $f = 0.3$ are displayed in figure 1. It is clearly seen that for this PC two complete PBGs exist, one between the second and third photonic bands and the other between the eighth and ninth photonic bands. The first PBG between the second and third photonic bands is pretty large. Its gap to midgap ratio is $\Delta\omega/\omega_g = 5.6\%$. The second PBG between the eighth and ninth photonic bands is quite small, with the gap to midgap ratio $\Delta\omega/\omega_g = 0.84\%$.

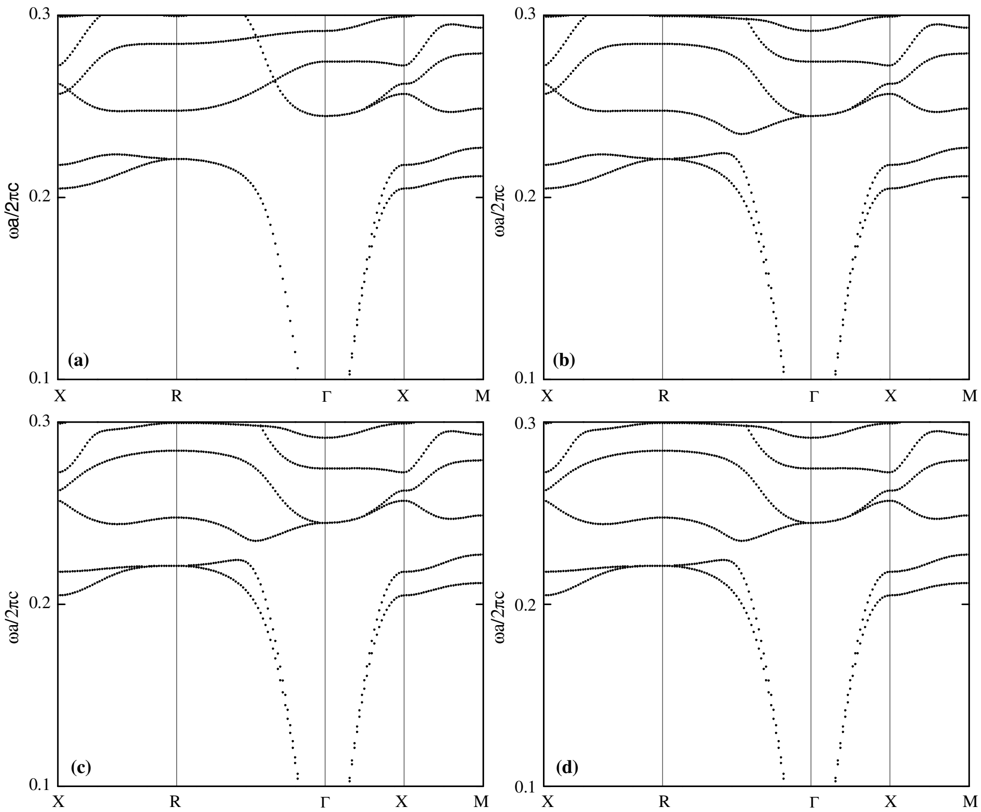

Figure 3. Calculated photonic band structures of a PC consisting of Te spheres in the sc lattice. The extraordinary axis of Te spheres is oriented along the [111] direction. The filling fraction of Te spheres is $f = 0.3$. As in figure 1, the photonic band structures of this PC in the whole Brillouin zone are plotted as a combination of four partial photonic band structures in the standard irreducible Brillouin zone of the sc lattice with the extraordinary axis of Te spheres oriented along (a) [111], (b) [$\bar{1}$11], (c) [1$\bar{1}$1], and (d) [11$\bar{1}$] directions. The high symmetry points in the irreducible Brillouin zone of the sc lattice are denoted by $\Gamma = (0, 0, 0)$, $X = (\pi/a)(1, 0, 0)$, $M = (\pi/a)(1, 1, 0)$, and $R = (\pi/a)(1, 1, 1)$.

The filling fraction of Te spheres is also one of the important factors to determine the existence of complete PBGs. In figure 2 the gap to midgap ratio of a PC consisting of Te spheres (with the extraordinary axis along the [111] direction) in the fcc lattice is plotted as a function of the filling fraction f of Te spheres. For the first PBG, defined by the second and third photonic bands, the gap to midgap ratio increases with the filling fraction for $f < 0.3$. At about $f = 0.3$, the gap to midgap ratio reaches a maximal value of 5.6%. For $f > 0.3$, the gap to midgap ratio decreases with the filling fraction. In addition, the complete bandgap between the second and third photonic bands exists in a rather wide range of filling fraction. In particular, it persists at a very low filling fraction of the birefringent spheres, adding considerably to the flexibility for realizing the tuning effect. The gap to midgap ratio of the second PBG decreases with the filling fraction. This PBG is closed when the filling fraction is larger than 0.4.

In the previous calculations, no complete PBG was found for PCs consisting of Te spheres arranged in the fcc, bcc, and sc lattices [8, 10]. In these calculations, the extraordinary axes of Te spheres are all aligned with the [100] direction. In our PCs, however, the extraordinary axes are oriented along the [111] direction. Thus, the orientation of the extraordinary axis of Te spheres plays an important role in the determination of the existence of complete PBGs. The creation of the partial and complete PBG by tuning the orientation of the birefringent spheres suggests a potential approach to achieve some degree of tunability of the photonic band structure through applying an external electric field, which rotates the extraordinary axis of the birefringent spheres relative to the PC structures.

The creation of the complete PBG is not limited to the fcc lattice that has a Brillouin zone closest to a sphere. To show this point, we also calculate the photonic band structures of a PC consisting of Te spheres in the sc lattice, whose Brillouin zone is obviously deviated from a sphere in comparison with the Brillouin zone of a fcc lattice. The results are shown in figure 3 for the case with the extraordinary axis of Te spheres oriented along the [111] direction of the sc lattice and the filling fraction of Te spheres $f = 0.3$. A complete PBG is found to appear between the second and third photonic bands. Its gap to midgap ratio is $\Delta\omega/\omega_{\mathrm{g}} = 3.3\%$. This again demonstrates the possibility of opening up a complete PBG by tuning the orientation of the extraordinary axis. We also study the dependence on the filling fraction of the PBG. Our results reveal that the behaviour of this dependence for sc PCs is similar to that of the first PBG for fcc PCs. At filling fraction $f \sim 0.3$, the gap to midgap ratio of the complete PBG is largest. Large or small filling fraction results in the closing of the complete PBG.

In summary, the photonic band structures of PCs consisting of birefringent dielectric spheres arranged in the fcc and sc lattice are studied by using a multiple-scattering method. Our results indicate the possibility of opening up complete PBGs in PCs of 3D simple lattices such as fcc and sc lattices by tuning the orientation of the extraordinary axis of birefringent spheres. The creation of the complete PBGs in the PCs also suggests some degree of tunability of the photonic band structure, provided that the extraordinary axis of all constituent birefringent spheres can be rotated while keeping the whole structure of the photonic system unchanged. The application of a strong external electric field may be a handle to achieve this tunability.

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