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The anisotropic photonic band gaps in three-dimensional photonic crystals with high-symmetry lattices composed of metamaterials and uniaxial materials

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ABSTRACT

In this paper, the properties of anisotropic photonic band gaps (PBGs) for three-dimensional (3D) photonic crystals (PCs) composed of tellurium (Te) spheres (the uniaxial materials) in homogeneous single-negative metamaterials (epsilon-negative materials) background with high-symmetry (simple-cubic) lattices are theoretically investigated based on the plane wave expansion method. The equations for calculating the anisotropic PBGs in the first irreducible Brillouin zone are theoretically deduced. The influences of the ordinary-refractive index, extraordinary-refractive index, filling factor of dielectric, the electronic plasma frequency, the dielectric constant of epsilon-negative materials on the anisotropic PBGs are also studied in detail, respectively, and some corresponding physical explanations are also given. The numerical results show that the anisotropic PBGs can be manipulated by the parameters as mentioned above. Introducing the uni-axial materials into 3D dielectric-epsilon-negative materials PCs can enlarge the PBGs, and also provide a way to obtain the complete PBGs as such kind of 3D PCs with high-symmetry lattices.

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1. Introduction

The photonic crystals (PCs) are structures with a periodically arranged the different dielectric materials. Since firstly proposed by Yablonovitch [1] and John [2], the PCs have attracted great attention due to their fascinating abilities to control the electromagnetic wave (EM wave) propagation. The PCs can provide the photonic band gaps (PBGs) [3–5] similar to the electronic band gaps in semiconductor, which originate from the interface of Bragg scattering in the periodic dielectric structure [6]. If the frequencies of EM wave are located in the PBGs, the propagation of EM wave is forbidden. The larger PBGs can be used to design several scientific and technical applications [7–10]. Recently, the metamaterials have been introduced into the PCs to realize the tunable PCs. The typical metamaterials PCs such as magnetic PCs [11-13], plasma PCs [14–16], superconductor PCs [17–19] and metallic PCs [20–22] have attracted the attention of researchers. Since the idea of metamaterials was firstly proposed by Veselago in 1967 [23], the

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metamaterials become a new active research field. In recently, the metamaterials have been realized in experiment by Smith et al. [24] and Pendry [25]. Pendry et al. [26,27] also investigated the negative refractive index of the metamaterials, and realized the metamaterials in the microwave frequency region. Compared to the conventional positive-index materials, the metamaterials reveal more interesting properties, such as inverse Snell's law, Cherenkov effects and reversed Doppler effect. As we know, the metamaterials can be divided into two categories. One configuration is named double-negative metamaterials whose permittivity ε and permeability μ are simultaneously negative [28]. However, the double-negative metamaterials hardly can be found in nature. The other category is called single-negative metamaterials [29]. The single-negative metamaterials also can be divided into two categories. One configuration, in which the permittivity is positive but the permeability is negative, gives rise to so-called mu-negative (MNG) materials. The other is that the permittivity is negative but the permeability is positive. In this case, the epsilon-negative (ENG) materials can be obtained. Fortunately, the ENG materials always can be found easily in nature, such as plasma, superconductor, semiconductor and metal. Therefore, the PCs containing the ENG materials can be used to design the omnidirectional reflector [30], multiple-channelled filter [31], tunable filter [32] and so on.







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Up to now, the one- and two-dimensional (2D) ENG materials PCs have been studied in detail, and have achieved rapid development in theoretical and experimental research [33-35]. Recently, the extensive works have been done on the 3D plasma PCs [36-38] and metal PCs. Those research results [34-38] showed that the tunable complete PBGs can be obtained as the ENG materials introduced, and the topology of 3D PC is a key factor to the existence of the PBGs. Especially, if 3D PCs have high-symmetry lattices, such as face-centered-cubic lattices [39], body-centered-cubic lattices [40] and simple-cubic (sc) lattices [40], the complete PBGs can hardly be achieved. In those cases, there are only the stop band gaps in the spectrum for a fixed direction of the incident light [39]. To overcome this drawback, the inserted dielectric constant of positive-index materials must be sufficiently large so that the resonant scattering of EM waves is prominent enough to open a complete band gap [39,40]. However, it is technically difficult to fabricate a high-symmetry 3D PCs composed of the ENG materials and large dielectric constant of dielectric. Therefore, to solve these problems, some methods have been reported: the symmetry reduction [41], introduced anisotropy in dielectric [42], or fabricating in a new topology, such as pyrochlore structure [43]. Among these methods, introduced anisotropic dielectric into PCs may be a good choose. As mentioned in the report of Li et al. [40], they introduced the tellurium (Te) into 3D dielectric PCs to obtain the complete PBGs. As we know, Te is a kind of the uniaxial materials. Thus, Te is a good candidate to be introduced into 3D PCs with high-symmetry lattices, which can obtain the complete PBGs.

The main purpose of this paper is to perform a systematic study of the anisotropic PBGs in 3D PCs with sc lattices doped by the anisotropic dielectric (uniaxial materials) and ENG materials based on a modified plane wave expansion (PWE) method. The proposed 3D PCs are that the dielectric spheres with the uniaxial materials are inserted in the ENG materials background periodically with sc lattices. The more general model of the ENG materials and the damping factor also are considered. This paper is organized as follows. The equations of computing the anisotropic PBGs for such 3D PCs are theoretically deduced in Section 2. In Section 3. the influences of the ordinary-refractive index. extraordinary-refractive index, filling factor, the electronic plasma frequency, the dielectric constant of the ENG materials on the anisotropic PBGs are explored, respectively. Finally, conclusions are given in Section 4. An $e^{i\omega t}$ time-dependence is implicit through the paper, with ω the angular frequency, t the time, and $i = \sqrt{-1}$. We also consider *c* is light speed in vacuum.

2. Theoretical model and numerical method

Schematic views of the 3D PCs with sc lattices containing the ENG materials and the first irreducible Brillouin zone showing symmetry point used for computing the anisotropic PBGs are plotted in Fig. 1. We assumed the radius of the sphere and lattice constant are *R* and *a* as shown in Fig. 1(a). Assumed the dielectric and the ENG materials are isotropic and homogeneous, and the relative dielectric functions are ε_a and ε_p , respectively. As we know, the ENG material is a kind of frequency-dependent dielectric, the dielectric function ε_p that meets the Drude model is written as the following [39]:

$$\varepsilon_p(\omega) = \varepsilon_b - \frac{\omega_p^2}{\omega(\omega + j\gamma)} \tag{1}$$

where ε_b , ω_p and γ are the dielectric constant of ENG materials, the electronic plasma frequency and the damping factor that contribute to the absorption and losses, respectively. In order to obtain the band diagrams of 3D PCs, several efficient numerical methods have been reported. The common methods are PWE [36], FDTD [44], scattering matrix [45], Dirichlet-to-Neumann map [46], plane-wavebased transfer-matrix [47], multidomain pseudospectral [48] and spectral element [49] methods. The PWE method is one of the most popular methods to compute the band structures. Especially, Kuzmiak and Maradudin [50] and Zhang et al. [51] proposed a modified PWE technique, which can calculate successfully the PBGs for the PCs composed of the Drude-type medium. As mentioned in Refs. [50,51], a standard linearization technique was used to solve the general nonlinear eigenvalue equation. In this paper, the same technique also will be used to obtain the anisotropic PBGs of 3D PCs with sc lattices composed of the ENG materials and the uniaxial materials [40].

As we know, the uniaxial material has two different principalrefractive indices known as ordinary-refractive and extraordinary-refractive indices, which can found in the nature. We consider the ordinary-refractive and extraordinary-refractive indices are n_o and n_e , respectively. For the anisotropic material, the dielectric constant ε_a is a dyadic and can be written as

$$\boldsymbol{\varepsilon}_{\mathbf{a}} = \begin{pmatrix} \varepsilon_{xx} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \varepsilon_{yy} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \varepsilon_{zz} \end{pmatrix}$$
(2)

where $\varepsilon_{xx} = n_x^2$, $\varepsilon_{yy} = n_y^2$, $\varepsilon_{zz} = n_z^2$. Therefore, for the uniaxial materials, the dielectric dyadic has only three cases for diagonal element permutation as [40] (a) $n_x = n_e$, $n_y = n_z = n_o$; (b) $n_y = n_e$, $n_x = n_z = n_o$; (c) $n_z = n_e$, $n_x = n_y = n_o$. We call them type-1, type-2 and type-3 uniaxial materials, respectively. In order to simplify, we just deduce the equations for obtaining the anisotropic PBGs of such 3D PCs doped by the type-1 uniaxial material. For the type-1 case, the ε_a^{-1} is the inverse dyadic of ε_a and can be written as

$$\boldsymbol{\varepsilon}_{\mathbf{a}}^{-1} = \begin{pmatrix} \varepsilon_{xx}^{-1} & 0 & 0\\ 0 & \varepsilon_{yy}^{-1} & 0\\ 0 & 0 & \varepsilon_{yy}^{-1} \end{pmatrix}$$
(3)



Fig. 1. Schematic structure of 3D ENG materials PCs with sc lattices. (a) 3D PCs structure, and (b) the first irreducible Brillouin zone showing symmetry point used for computing the band structures.

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