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Study of bandgap characteristics of three-dimensional photonic crystal with typical structures

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ABSTRACT

The aim of this study was to investigate the bandgap characteristics of three-dimensional photonic crystals of SIC, GaP, InP, GaAs, InAs, InSb, HgTe, and HgSe materials with typical structures under the following different conditions: diamond, face-centered cubic (fcc), and wood. Based on the plane wave expansion method, the influence of factors such as the dielectric constant, density on the upper and lower boundary, and width on the bandgap characteristics of three-dimensional photonic crystals was studied, in addition to the influence of factors such as the filling ratio and the radius of the ball on the bandgap variation in three-dimensional photonic crystals. The results show that the bandgap width of diamond and fcc structures can be improved by increasing the dielectric constant and density. However, the bandgap width of wood structures decreases, as they have wider photonic bandgaps when the filling rate is 0.325 and the ball radius is highly symmetrical. These results provide the theoretical basis for the design of three-dimensional photonic crystal devices.

1. Introduction

The concept of photonic crystals was proposed by John [1] and Yablonovich [2] in 1987. They are novel materials with photonic bandgaps, and some frequencies in this bandgap can become forbidden. These properties enable their use in optical communication devices, electromagnetic wave transmission devices, the microstructure of electromagnetic transmission devices, and optical energy devices, in addition to filters, absorbers, and electromagnetic waveguides [3–7]. Different devices are designed to meet the requirement for the propagation of electromagnetic wave frequencies by changing the photonic crystal structure, material parameters, filling ratio, etc. [8–15]. Photonic crystals are categorized into one-dimensional, two-dimensional, and three-dimensional photonic crystals with a periodic structure. Although one- and two-dimensional photonic crystal structures control the guiding of light, three-dimensional photonic crystal structures with a complete bandgap have the most potential in several aspects. Many published papers have only focused on the bandgap characteristics in a single material; the characteristic of frequencies with upper and lower boundaries has been reported scarcely.

In this paper, we designed three-dimensional photonic crystals with typical structures under different conditions, diamond, face-centered cubic (fcc), and wood, and we also studied the bandgap characteristics by changing the material parameters, photonic crystal structure, and filling ratio. Moreover, we obtained the bandgap characteristics of frequencies with upper and lower boundaries.

The paper is organized as follows: In Section 2, the plane wave expansion method is introduced. In Section 3, the bandgap characteristics of the three-dimensional photonic crystal are calculated, and the characteristics of frequencies with upper and lower boundaries are analyzed. Finally, conclusions are presented in Section 4.

2. Theoretical method

The bandgap characteristics of three-dimensional photonic crystals were solved using the plane wave expansion method. This method was developed for plane waves, and Maxwell's equations of the propagation electromagnetic wave were converted into an eigen equation. We can obtain the eigenfrequency of the three-dimensional photonic crystals by solving the eigen equation. The eigen equation can be represented as follows:

$$-\sum_{\rightarrow G'} K(\vec{G}-\vec{G}')(\vec{k}+\vec{G}')\times((\vec{k}+\vec{G})\times\rightarrow E_{\rightarrow kn}(\rightarrow G')) = \frac{{\omega_{kn}}^2}{c^2}\rightarrow E_{kn}(\vec{G}) \quad (1)$$

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$$-\sum_{\to G'} K(\vec{G}-\vec{G}')(\vec{k}+\vec{G})\times((\vec{k}+\vec{G})\times\to H_{\to kn}(\to G'\,)) = \frac{{\omega_{kn}}^2}{c^2}\to H_{kn}(\vec{G}) \tag{2}$$

In Eqs. (1) and (2), where $\vec{k}$ denotes the wave vectors and $\vec{G}$ the reciprocal lattice vector, $\dot{E}_{kn}(\vec{G})$ and $\dot{H}_{kn}(\vec{G})$ are the coefficient for the plane electromagnetic wave of the electric and magnetic fields. The eigenvalue of the equation is obtained based on Eqs. (1) and (2), in addition to the dispersion coefficient $\omega(\vec{k})$. Based on the changing direction of $\vec{k}$, the bandgap characteristics of the three-dimensional photonic crystal were achieved by calculating the relation between $\dot{E}_{kn}(\vec{G})$ and $\dot{H}_{kn}(\vec{G})$.

3. Results and discussion

3.1. Material characteristics of three-dimensional photonic crystal with diamond, fcc, and wood structure

Three-dimensional photonic crystals of SIC, GaP, InP, GaAs, InAs, InSb, HgTe, and HgSe materials with typical structures under different conditions, diamond, fcc, and wood, are presented in Table 1. The material characteristics of the dielectric constant, density (10^{-3} kg), melting point (°C), lattice structure, and material race are also introduced in Table 1. From Table 1, we know that the dielectric constant and density of eight materials gradually increase, the biggest difference of the dielectric constant is eight, the biggest difference of the density is 2.5751 (10^{-3} kg), the melting point of eight materials gradually decrease, the melting point of GaAs and HgTe changes slightly, and the lattice structure is sphalerite. The materials are IV race (SIC), III–V race (GaP, InP, GaAs, InAs, and InSb), and II–VI (HgTe and HgSe) semiconductor materials.

3.2. The dielectric constant has an effect on the complete bandgap of the diamond, fcc, and wood structures

Based on the plane wave expansion method, we calculated the bandgap characteristics of three-dimensional photonic crystals of SIC, GaP, InP, GaAs, InAs, InSb, HgTe, and HgSe materials with typical structures under different conditions, such as diamond, fcc, and wood, at a filling rate of 0.325; these results are shown in Fig. 1. The abscissa represents the dielectric constant, and the ordinate represents the bandgap of the upper and lower boundaries. From Fig. 1, we know that the upper- and lower-boundary frequencies of the fcc structure are the highest, the diamond structure second, and the wood structure the lowest.

They have something in common: the bandgap of the upper- and lower-boundary frequency decreases with increasing dielectric constant. We also know that the difference is the change in the width of the bandgap, as shown in Fig. 1b. The abscissa represents the dielectric constant, and the ordinate represents the bandwidth of the gap. From Fig. 1b, we know that the diamond structure forms a wider bandgap of 0.1547 Hz, with the bandwidth ranging from 0.3683 to 0.523 Hz for the HgSe material; the bandgap characteristics of this structure are shown in Fig. 2. From Fig. 3, we know that the wood structure for the HgSe material forms a narrow bandgap of 0.0257 Hz, with the bandwidth ranging from 0.051 to 0.076 Hz. From Fig. 3b, we also know that the bandwidth of the gap for the wood structure is higher than that for the fcc structure with the dielectric constant ranging between 9.72 and 14.55, but the

Table 1
Material characteristics of three-dimensional photonic crystals with diamond, fcc, and wood structures [16].

Materials	Dielectric constant	Density (10^{-3} kg)	Melting point (°C)	Lattice structure	Race
SIC	9.72	3.2	2830	Sphalerite	IV
GaP	11.1	4.1297	1467	Sphalerite	III–V
InP	12.35	4.787	1070	Sphalerite	III–V
GaAs	13.18	5.307	1238	Sphalerite	III–V
InAs	14.55	5.667	943	Sphalerite	III–V
InSb	17.72	5.7751	525	Sphalerite	III–V
HgTe	20	8.2	670	Sphalerite	II–VI
HgSe	25	8.26	800	Sphalerite	II–VI

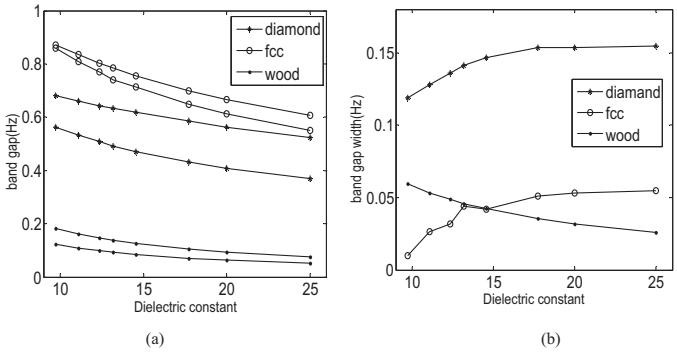

Fig. 1. The complete forbidden band characteristics of diamond, fcc, and wood structures with SIC, GaP, InP, GaAs, InAs, InSb, HgTe, and HgSe: (a) relationship between the bandgap of the upper and lower boundary and the dielectric constant. (b) Relationship between the band width and the dielectric constant.

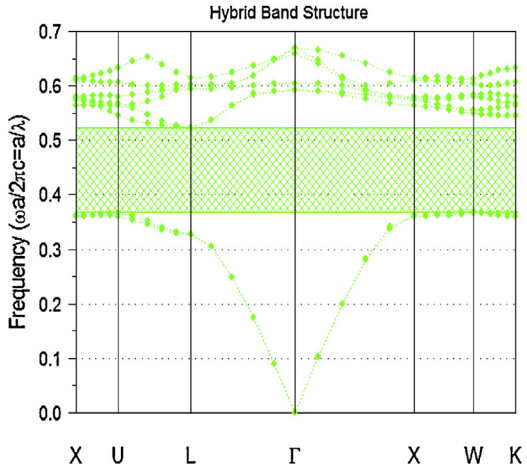

Fig. 2. The bandgap characteristics of diamond structures with HgSe materials.

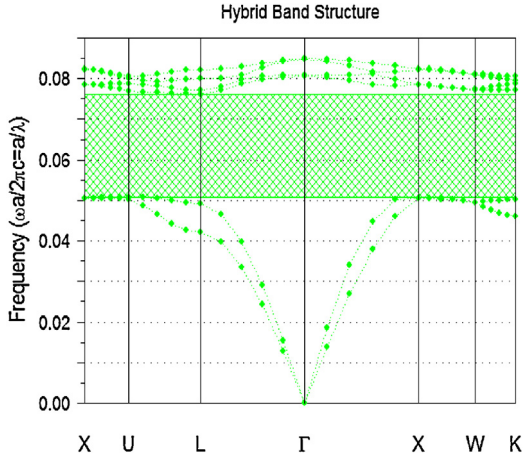

Fig. 3. The bandgap characteristics of wood structures with HgSe materials.