

Fibonacci Sequences Quasiperiodic $A^5B^6C^7$ Ferroelectric Based Photonic Crystal: FDTD analysis

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Abstract

In this study, we present an investigation of the optical properties and band structures for the conventional and Fibonacci photonic crystals (PCs) based on some $A^5B^6C^7$ ferroelectrics (SbSBr and BiTeCl). Here, we use one dimensional SbSBr and BiTeCl based layers in air background. We have theoretically calculated the photonic band structure and transmission spectra of SbSBr and BiTeCl based PC superlattices. The position of minima in the transmission spectrum correlates with the gaps obtained in the calculation. The intensity of the transmission depths is more intense in the case of higher refractive index contrast between the layers. In our simulation, we employed the finite-difference time domain technique and the plane wave expansion method, which implies the solution of Maxwell equations with centered finite-difference expressions for the space and time derivatives.

1. Introduction

Photonic crystals (PhCs) are structured dielectric composites that are designed and fabricated to have periodic optical properties that strongly alter the properties and propagation of light. One of the defining properties of PhCs is photonic band gaps – frequency ranges where light cannot propagate because of the destructive interference between coherent scattering paths. We can observe the same situation in the PhCs based superlattices [1,2]. The structures intermediate between the periodic and disordered structures (quasiperiodic structure) - the Fibonacci and Thue-Morse superlattices, occupy a special place among the superlattices. The strong resonances in spectral dependences of fractal multilayers can localize light very effectively. In addition, long-range ordered aperiodic photonic structures offer extensive flexibility for the design of optimized light emitting devices, the theoretical understanding of the complex mechanisms governing optical gaps, and mode formation in aperiodic structures becomes increasingly more important. The formation of photonic band gaps and the existence of quasi-localized light states have already been demonstrated for one (1D) and two-dimensional (2D) aperiodic structures based on Fibonacci and the Thue-Morse sequences [2]. The unusual electron properties of quasiperiodic potentials have also stimulated extensive

research of the optical counterparts. However, to the best of our knowledge, a rigorous investigation of the band gaps and optical properties in the more complex types of aperiodic structures has not been reported so far.

In this paper, we investigated the energy spectrum and optical properties in the Fibonacci-type photonic band gap (PBG) structures consisting of ferroelectric material (SbSBr and BiTeCl) [3] in detail by using the finite-difference time-domain (FDTD) method and the plane wave expansion method (PWE). The choice of the SbSBr and BiTeCl crystals as the active media for our investigation were associated with their unusual optical and electronic properties. It is well known that SbSBr and BiTeCl are the ferroelectric material and their properties are very sensitive to external influences (temperature, electric field, stress, and light) [3].

2. Computational Details

2.1. Fibonacci Sequences and Model

Quasiperiodic structures are nonperiodic structures that are constructed by a simple deterministic generation rule. In a quasiperiodic system, two or more incommensurate periods are superimposed so that it is neither aperiodic nor a random system and, therefore, can be considered as intermediate the two [1]. In other words, due to a long-range order, a quasiperiodic system can form forbidden frequency regions called pseudo band gaps similar to the band gaps of a PC and simultaneously possess localized states as in disordered media [2]. The Fibonacci multilayer structure (well-known quasiperiodic structure) has been studied in the past decade, and recently the resonant states at the band edge of the photonic structure in the Fibonacci sequence are studied experimentally, too [4]. A 1D quasiperiodic Fibonacci sequence is based on a recursive relation, which has the form, $S_{j+1}=\{S_{j-1}, S_j\}$ for $j \gg 1$, with $S_0=\{A\}$, $S_1=\{B\}$, $S_2=\{AB\}$, $S_3=\{BAB\}$, $S_4=\{ABBAB\}$ and soon, where S_j is a structure obtained after j iterations of the generation rule [1]. Here, A and B are defined as being two dielectric materials, with different refractive indices (n_A, n_B) and have geometrical layer thickness (d_A, d_B). In place of materials A and B, we used air for A for material and

BiTeCl [5] and SbSBr [6] for B material. In Fig. 1 (a) and (b), we schematically show the geometry of Conventional Photonic Crystal (CPCs) and Fibonacci Photonic Crystal (FPCs). The typical 1D CPCs and FPCs are shown in Fig.1. The thickness of the considered layers of A and B are $d_A = 0.5a$ and $d_B = 0.5a$, respectively. The lattice constant is $a = (d_A + d_B) = 1 \mu\text{m}$. The filling fraction f is the ratio between the thickness of the lower refractive index layer (air) and the period of the PC, i.e. $f = d_A/(d_A + d_B)$. The filling fraction is set to 0.5. The refractive index contrasts of BiTeCl and SbSBr are taken as shown in Ref [5] and [6]. The refractive index of the background dielectric medium is assumed as air ($n_{\text{air}}=1.0$).

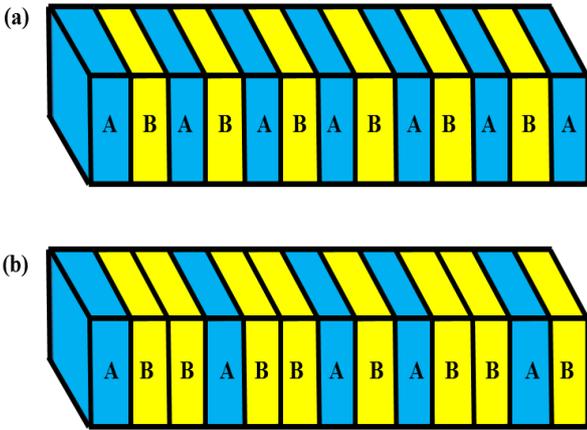


Figure 1: 1-Dimensional Conventional Photonic Crystal Structure (a) and Fibonacci Photonic Crystal Structure (b).

2.2. Finite Difference Time Domain (FDTD) Method and Plane Wave Expansion Method (PWE)

In our calculations, we used the OptiFDTD software package [7]. The OptiFDTD software package is based on the finite-difference time-domain (FDTD) method for transmission spectra and the plane wave expansion method (PWE) for the photonic band structure.

The photonic band structures of the proposed PCs were calculated by solving the Maxwell equations. The Maxwell equation in a transparent, time-invariant, source free, and non-magnetic medium can be written in the following form:

$$\nabla \times \frac{1}{\epsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) = \frac{\omega^2}{c^2} \mathbf{H}(\mathbf{r}) \quad (1)$$

Where,

$\epsilon(\mathbf{r})$ is the space dependent dielectric function

c is the speed of light in vacuum.

$\mathbf{H}(\mathbf{r})$ is the magnetic field vector of frequency ω and time dependence $e^{j\omega t}$.

This equation is sometimes called the Master Equation, and represents a Hermitian eigen-problem, which would not be applicable if the wave equation were derived in terms of the

electric field. The Bloch theorem states that, due to infinite periodicity, the magnetic field will take the form:

$$\mathbf{H}(\mathbf{r}) = e^{j\mathbf{k}\mathbf{r}} \mathbf{h}_{\mathbf{k}}(\mathbf{r}) \quad (2)$$

Where

$$\mathbf{h}_{\mathbf{k}}(\mathbf{r}) = \mathbf{h}_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) \quad (3)$$

for all combinations of lattice vectors \mathbf{R} . Thus, Maxwell equation is given in operator form:

$$(\nabla \times j\mathbf{k}) \times \left[\frac{1}{\epsilon(\mathbf{r})} (\nabla \times j\mathbf{k}) \right] \times \mathbf{h}_{\mathbf{k}} = \frac{\omega^2}{c^2} \mathbf{h}_{\mathbf{k}} \quad (4)$$

By solving these equations for the irreducible Brillouin zone, we can obtain the photonic band structure.

FDTD algorithm is one of the most appropriate calculation tools [8]. For solving Maxwell's equations, depending on the time, the FDTD algorithm divides the space and time in a regular grid. Perfect matched layers (PMLs) can be used in the determination of the boundary conditions [9]. In general, the thickness of the PML layer in the overall simulation area is equal to a lattice constant. FDTD solves the electric and magnetic fields by rating depending on space and time, and deploys that rating in different spatial regions by sliding each field component half a pixel. This procedure is known as Yee grid discretization. Fields in these grids can be classified as Transverse Magnetic (TM) and Transverse Electric (TE) polarization. In our calculations, we have used Perfect Magnetic Conductor (PMC) and Anisotropic Perfectly Matched Layer (APMLs) boundary conditions at the x- and z-directions, respectively.

3. Results and Discussion

3.1. Photonic Band Structure and Transmittance

We calculate the spectral properties up to n th generations ($n=10$) Fibonacci-type quasi-periodic layered structures consisting of BiTeCl and SbSBr compounds. Band structure of 1D of BiTeCl and SbSBr based CPCs have been calculated in high symmetry directions in the first Brillouin zone (BZ) and shown in Fig. 2(a,b). As seen in Fig 2(a), there are three photonic band gaps (PBGs) for BiTeCl compound. The width of the PBGs are (51-85) THz for first, (118-166) THz for the second, (198-236) THz for the third, respectively. On the other hand, for SbSBr compound, the first TE band gaps appeared to be between the first and second bands in the frequency ranges (52-87) THz, the second band gaps (122-170) THz, and the third band gaps (205-241) THz. When the frequency of the incident electromagnetic wave drops in these PBGs, the electromagnetic wave will be reflected completely by the photonic crystal. It can be seen in Fig. 2, transmittance is zero in these range of frequencies where the refractive index of the structure is positive and the spectral width of the gaps are invariant with the change in the transmittance (Tables 1 and 2).

The numerical results of variation of full band gap with changing filling factor from 0.1 up to 0.9 is given in Tables

1 and 2. Variation of band gap sizes (%) as a function of filling factor changes between 4 and 35 for TE1 band of both types of crystals. The largest gap sizes are approx. 35% for BiTeCl when filling factor is as high as 0.2. On the other hand, the largest gap sizes are approx. 34% for SbSBr when the filling factor is as high as 0.7. Then, it decreases when the filling factor continues to increase for both crystals. On the other hand, the second and third band gap sizes do not change too much according to the filling factor.

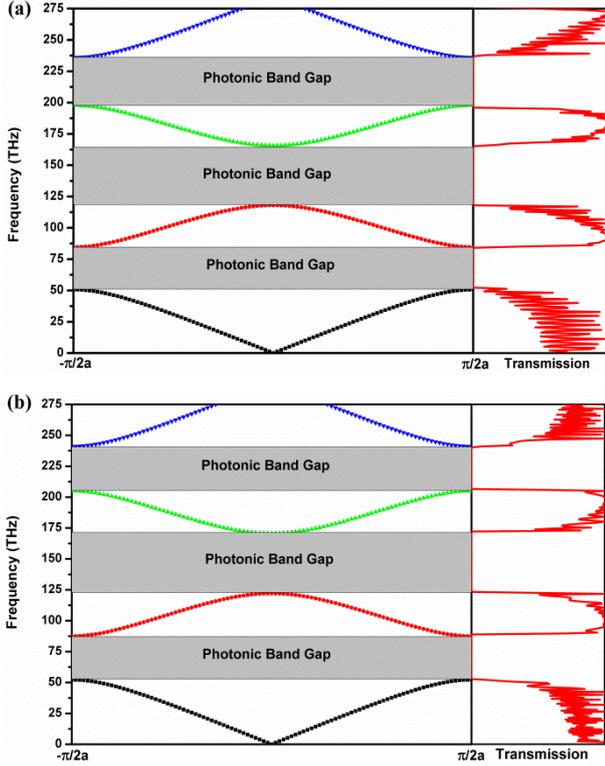


Figure 2: TE Band structure and transmittance spectra of BiTeCl (a) and SbSBr (b) in 1D.

Table 1: Variation of full band gap size for TE modes with filling factor for BiTeCl based layers in air background.

Filling Factor	TE1		TE2		TE3	
	Band Gap (THz)	Gap Size (%)	Band Gap (THz)	Gap Size (%)	Band Gap (THz)	Gap Size (%)
0.1	(86-148)	26.49	(205-287)	16.66	(347-400)	7.09
0.2	(68-139)	34.29	(196-220)	5.76	(280-341)	9.82
0.3	(59-120)	34.07	(167-196)	7.98	(246-292)	8.55
0.4	(54-100)	29.87	(136-186)	15.52	(235-243)	1.67
0.5	(51-85)	25.00	(118-166)	16.90	(198-236)	8.75
0.6	(49-73)	19.67	(106-145)	15.53	(173-215)	10.82
0.7	(48-	14.28	(99-	12.77	(156-	10.08

0.8	(64-57)	9.61	(128-114)	9.09	(191-171)	7.88
	(47-51)		(94-103)		(141-154)	
0.9	(47-51)	4.08	(94-103)	4.56	(141-154)	4.40

Table 2: Variation of full band gap size for TE modes with filling factor for SbSBr based layers in air background.

Filling Factor	TE1		TE2		TE3	
	Band Gap (THz)	Gap Size (%)	Band Gap (THz)	Gap Size (%)	Band Gap (THz)	Gap Size (%)
0.1	(48-53)	4.95	(96-106)	4.95	(145-159)	4.60
0.2	(48-59)	10.28	(98-118)	9.25	(150-176)	7.97
0.3	(49-66)	14.78	(102-132)	12.82	(161-197)	10.05
0.4	(50-75)	20.0	(110-150)	15.38	(179-221)	10.50
0.5	(52-87)	25.17	(122-170)	16.43	(205-241)	8.07
0.6	(55-103)	30.37	(141-190)	14.80	-	-
0.7	(61-123)	33.69	(174-198)	6.45	(250-302)	9.42
0.8	(70-141)	33.64	(198-230)	7.47	(290-346)	8.80
0.9	(90-149)	24.68	(209-277)	13.99	(349-415)	8.63

Then, we have calculated the transmission spectra of Conventional and Fibonacci types photonic crystals with unit cells composed by SbSBr and BiTeCl and the same optical thickness for each layer. The spectra are shown in Figures 3-8. The position of the minima in the transmission spectrum correlates with the gaps obtained in the calculation. The intensity of the transmission depths is more intense in the case of higher refractive index contrast between the layers. This phenomenon is even more clear for Fibonacci structures (see, Figs. 3-8). In Figures 4-8, we plot the overall transmission as a function of the incidence angle (0° - 75°). In this case, we observed that, for lower refractive index contrast, the overall transmission is higher for Fibonacci structures, while for a higher refractive contrast the overall transmission is higher for conventional crystals.

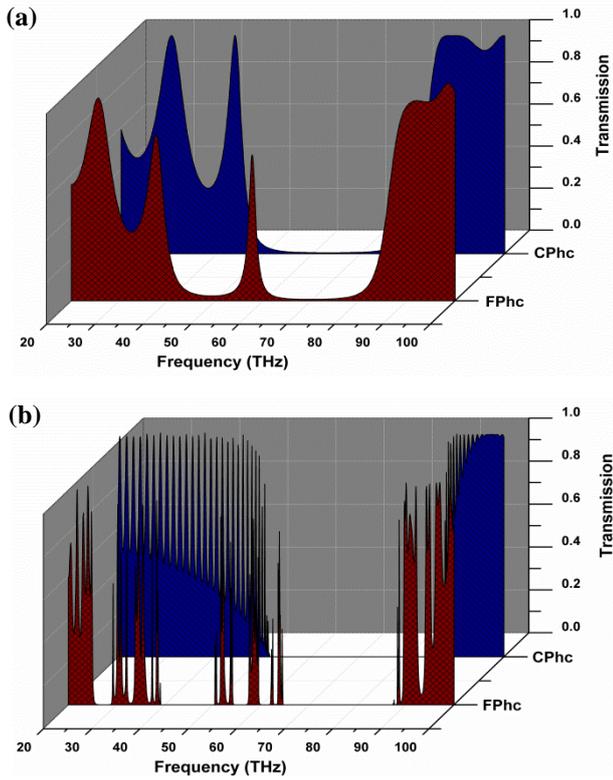


Figure 3: TE Transmittance spectrum of BiTeCl based Conventional and Fibonacci Photonic crystal structures of (a) 5th and (b) 10th generations.

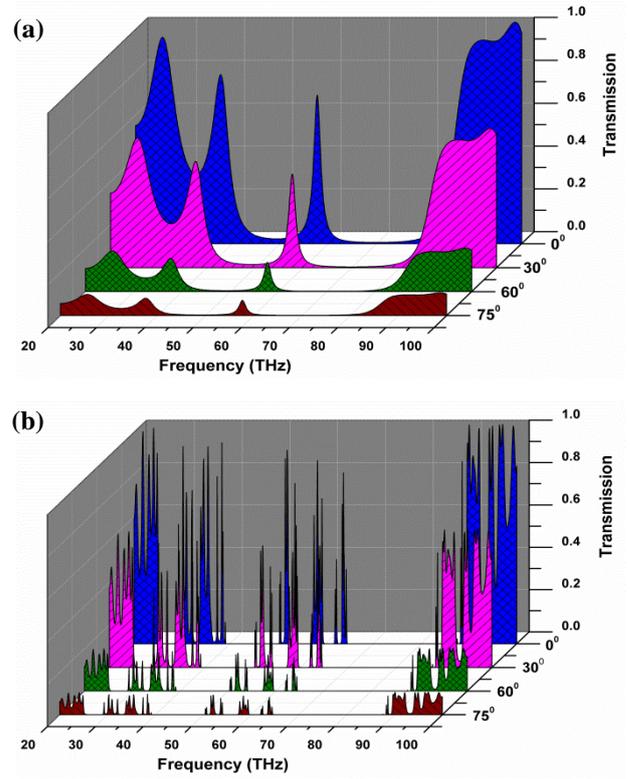


Figure 5: TE Transmittance spectrum of BiTeCl based Fibonacci Photonic crystal structures of (a) 5th and (b) 10th generations from 0° to 75° .

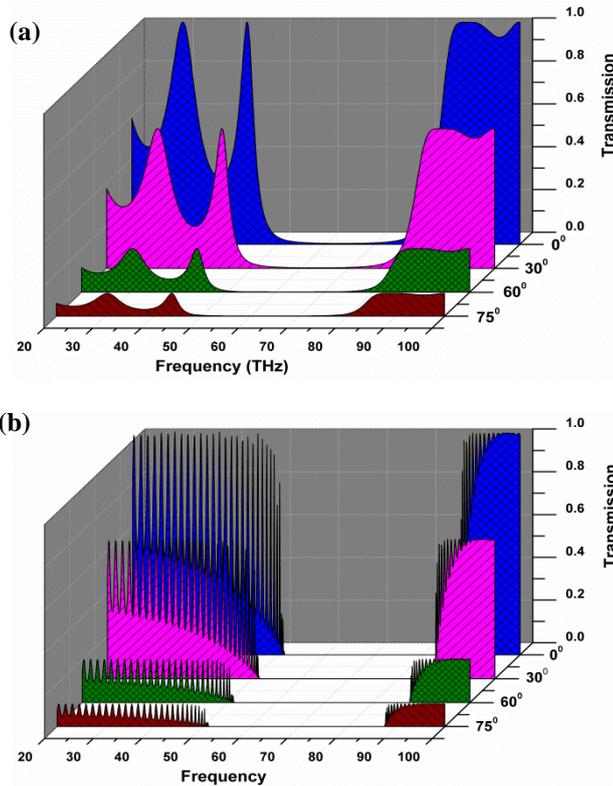


Figure 4: TE Transmittance spectrum of BiTeCl based Conventional Photonic crystal structures of (a) 5th and (b) 10th generations from 0° to 75° .

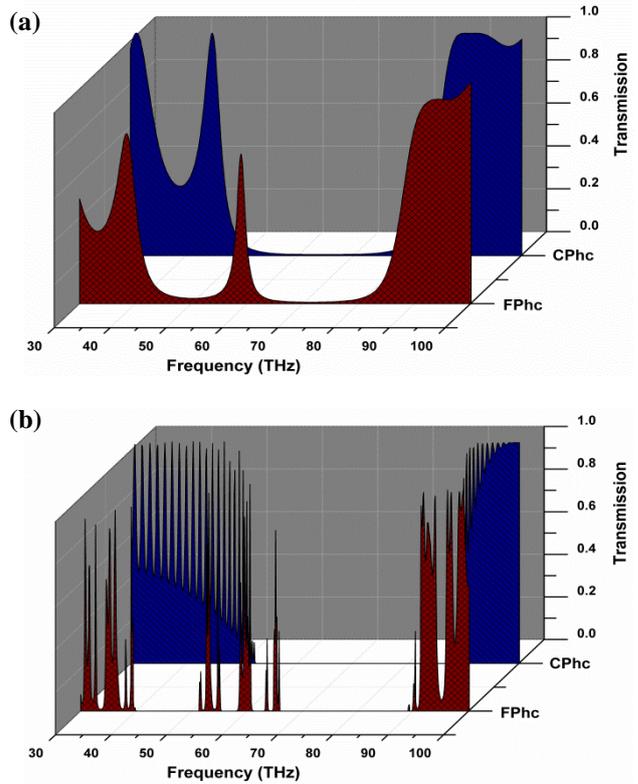


Figure 6: TE Transmittance spectrum of SbSBr based Conventional and Fibonacci Photonic crystal structures of (a) 5th and (b) 10th generations.

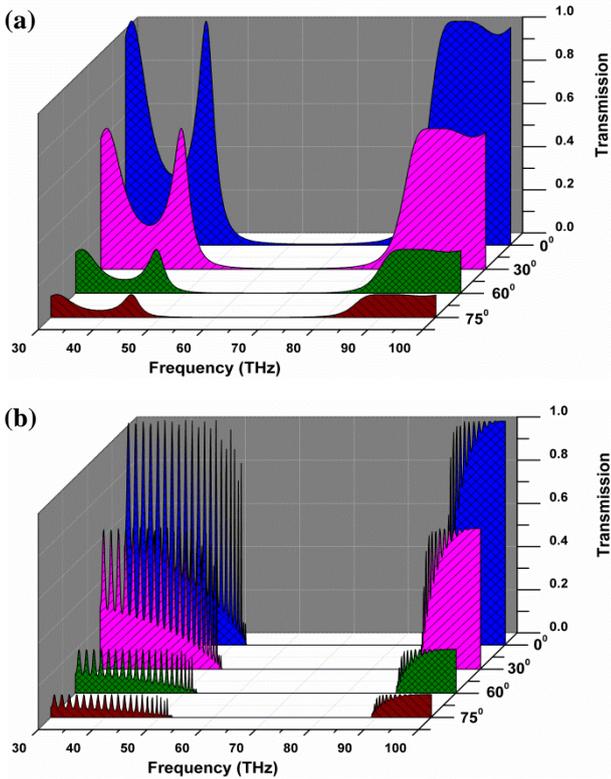


Figure 7: TE Transmittance spectrum of SbSBr based Conventional Photonic crystal structures of (a) 5th and (b) 10th generations from 0° to 75° .

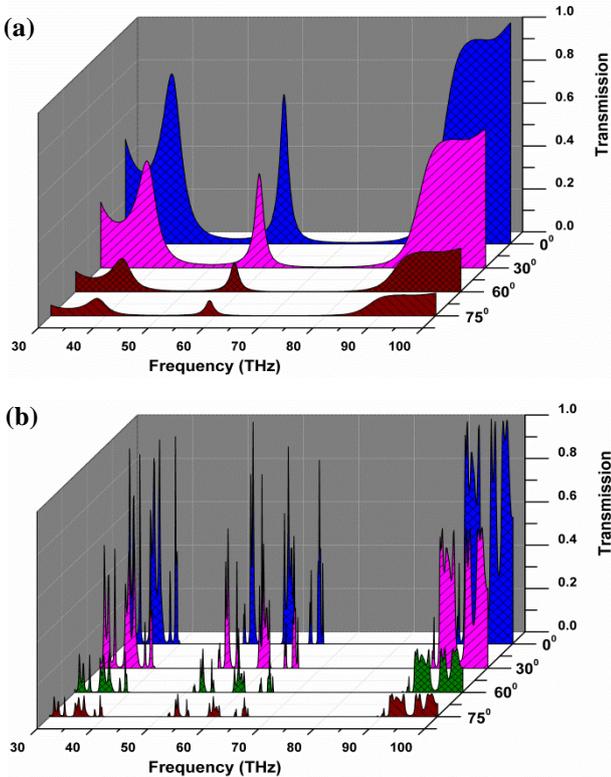


Figure 8: TE Transmittance spectrum of SbSBr based Fibonacci Photonic crystal structures of (a) 5th and (b) 10th generations from 0° to 75° .

4. Conclusions

The photonic band structures and transmission properties of the 1D BiTeCl and SbSBr based conventional PCs and Fibonacci PCs consisting of layers immersed in air were studied. We have investigated the band structure and transmittance spectra of BiTeCl and SbSBr based CPhc and FPhc. Through the theoretical analysis of the transmission spectrum, it was found that the number of transmission peaks of a Fibonacci structure is in the law of $M_n = M_{n-1} + M_{n-2}$ in accordance with the structure of FPhc where M_n represents the number of transmission peaks of an FPhc with the n series. The results show that the number of the repetition period also has a great influence on the average transmittance of the pass band of both conventional and Fibonacci PCs.

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