

# $A^I B^{III} C^{VI}_2$ (A = Cu, Ag; B = Ga, In; C = S, Se, Te) based photonic crystal superlattices: Optical properties

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In this study, we present an investigation of the optical properties and band structures for the photonic structures based on  $A^I B^{III} C^{VI}_2$  with a Fibonacci sequence that can act as a multi-wavelength birefringent filter. The filtering wavelengths are analyzed by the indices concerning the quasi-periodicity of a Fibonacci sequence and the average

lattice parameter. The transmittances of filtering wavelengths can be tuned by varying structure parameters such as the lengths of poled domains, filling factor, and dispersion relation. In our simulation, we employed the finite-difference time domain (FDTD) technique, which implies a solution from Maxwell equations.

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**1 Introduction** Photonic crystals (PCs) are structures with periodically modulated refractive indices whose distribution follows the periodicity of order of a fraction of the optical wavelength. They can generate spectral regions named stop (photonic) bandgaps where light cannot propagate in a manner analogous to the formation of electronic band gaps in dielectrics. The physical properties of a new class of artificial crystals, the so-called quasi-periodic structures, have also attracted a lot of interest in recent decades [1, 2]. Quasi-periodic systems can be considered as suitable models to describe the transition from the perfect periodic structure to the random structure. In this, the transmission properties and band structure of the one (1D) – dimensional ternary compounds of the  $A^I B^{III} C^{VI}_2$  family (A = Ag, Cu; B = In, Ga, Al; C = Se, Te, S) multilayer system built according to the generalized Fibonacci sequence will be considered. The FDTD method is then used in our study [3]. It is well known that the ternary compounds of the  $A^I B^{III} C^{VI}_2$  family are very useful nonlinear optical materials in a wide optical range from 0.7 to 20  $\mu\text{m}$  [4]. They have interesting properties for the implementation of active PCs and have the advantage of a wide electro-optic coefficient and low loss optical propagation in the mid IR region [5]. Due to their high electro-optical,

acousto-optical, and nonlinear coefficients,  $A^I B^{III} C^{VI}_2$  represents an excellent candidate for the realization of dynamic PC structures [6].

In this article, we study the 1D photonic crystal superlattices of the  $A^I B^{III} C^{VI}_2$  compounds.

## 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 between 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 [3]. A 1D quasi-periodic Fibonacci sequence is

based on a recursive relation. Let us now consider a quasiperiodic multilayer based on the Fibonacci sequence. The Fibonacci numbers,  $F_j$  with  $j=0, 1, 2, 3 \dots$ , characterized by the relation  $F_{j+1}=F_j+F_{j-1}$ , with  $F_0=0$  and  $F_1=1$  and so  $\{F_j\}=\{0, 1, 1, 2, 3, 5, 8, 13, 21, \dots\}$ . Thus, each number in the sequence is just the sum of the preceding two number. In a similar manner, we have constructed the Fibonacci sequences based on a recursive relation which has the form,  $F_{j+1}=\{F_{j-1}, F_j\}$  for  $j > 1$ , with  $F_0=\{B\}$ ,  $F_1=\{A\}$ ,  $F_2=\{BA\}$ ,  $F_3=\{ABA\}$ ,  $F_4=\{BAABA\}$  and so on, where  $F_j$  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 material and A<sup>I</sup>B<sup>III</sup>C<sup>VI</sup><sub>2</sub> (A = Cu, Ag; B = Ga, In; C = S, Se, Te) compounds for B material.

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 Photonic crystal ( $a$ ), i.e.,  $f = d_A / (d_A + d_B)$ . The filling fraction is set to 0.5 for both the band structure and transmittance spectra calculations. The refractive index of anisotropic A<sup>I</sup>B<sup>III</sup>C<sup>VI</sup><sub>2</sub> materials are taken from Refs. [7, 8] and are given in Table 1. The refractive index of the background dielectric medium is assumed as air ( $n_{\text{air}} = 1.0$ ).

**2.2 Finite difference time domain (FDTD) method and plane wave expansion method (PWE)** In our calculations, we used OptiFDTD software package [9]. 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 a 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:

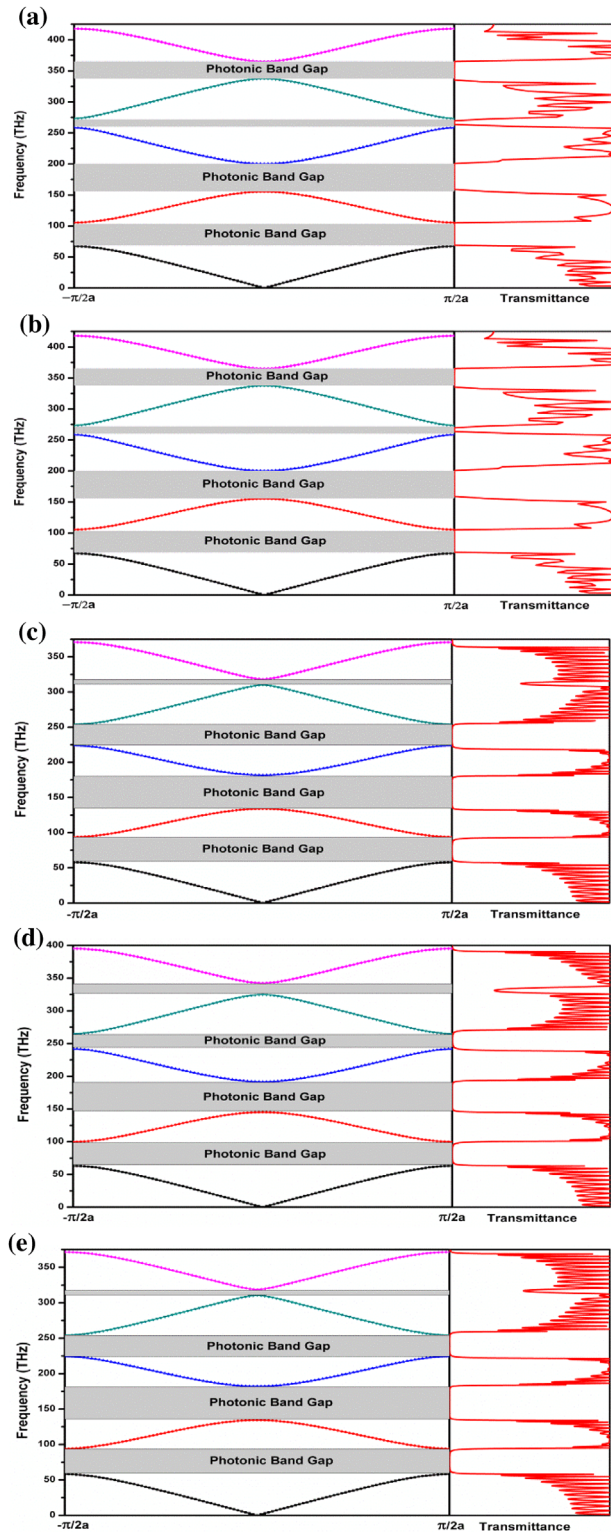
$$\nabla \times \frac{1}{\varepsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) = \frac{\omega^2}{c^2} \mathbf{H}(\mathbf{r}) \quad (1)$$

where,  $\varepsilon(\mathbf{r})$  is the space dependent dielectric function,  $c$  is

**Table 1** The refractive index of A<sup>I</sup>B<sup>III</sup>C<sup>VI</sup><sub>2</sub> materials.

material	$n_x (=n_o)$	$n_y (=n_o)$	$n_z (=n_e)$	$*\lambda$ ( $\mu\text{m}$ )	ref.
AgGaS <sub>2</sub>	2.408	2.408	2.355	0.6	[7]
AgGaSe <sub>2</sub>	2.617	2.617	2.586	0.6	[7]
AgInSe <sub>2</sub>	2.7971	2.7971	2.8453	1.10	[7]
CuGaS <sub>2</sub>	2.5681	2.5681	2.5630	0.90	[8]
CuInS <sub>2</sub>	2.7907	2.7907	2.7713	0.90	[8]

\* $\lambda$  = wavelength, at which the refractive index is measured



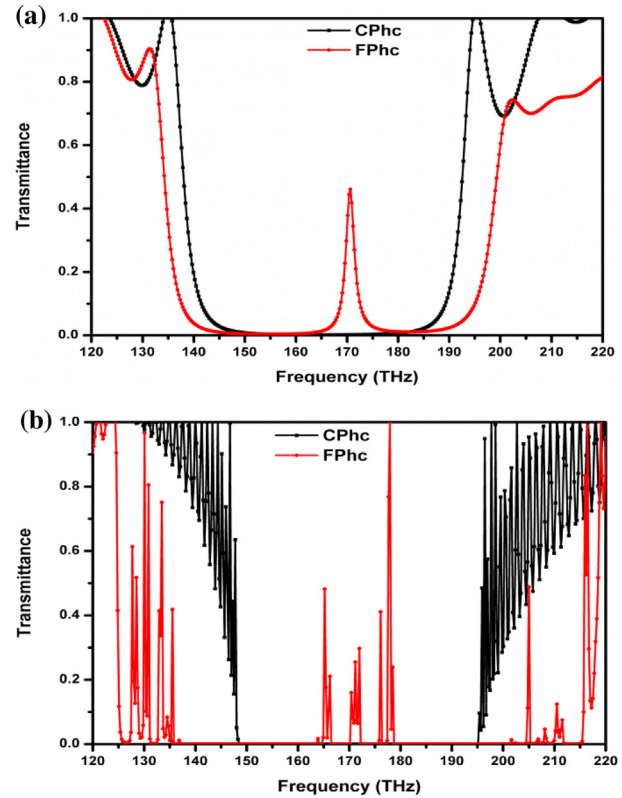
**Figure 1** TE Band structure and transmittance spectra of A<sup>I</sup>B<sup>III</sup>C<sup>VI</sup><sub>2</sub> based CPhc in 1D. AgGaS<sub>2</sub> (a), AgGaSe<sub>2</sub> (b), AgInSe<sub>2</sub> (c), CuGaS<sub>2</sub> (d), and CuInS<sub>2</sub> (e).

the speed of light in vacuum, and  $\mathbf{H}(\mathbf{r})$  is the magnetic field vector of frequency  $\omega$  and time dependence  $e^{i\omega t}$ .

By solving this equation for the irreducible Brillouin zone, we can obtain the photonic band structure.

FDTD algorithm is one of the most appropriate calculation tools [10]. For solving Maxwell's equations depending on the time, FDTD algorithm divides the space and time in a regular grid.

**3 Results and discussion** The calculated band structures and transmittance spectra of 1D  $A^{III}B^{III}C^{VI}_2$  based CPhc in high symmetry directions in the first Brillouin zone (BZ) are shown in Fig. 1(a, b, c, d, and e). We can see that there are four photonic band gaps (PBG) for  $A^{III}B^{III}C^{VI}_2$  based CPhc from Fig. 1(a, b, c, d, and e). The width of the PBGs are (67–105) THz for first, (155–200) THz for the second, (258–273) THz for the third, and (337–365) THz for the fourth for  $AgGaS_2$ , respectively. On the other hand, for  $AgGaSe_2$ , the first TE band gaps appeared to be between the first and second bands in the frequency ranges of (61–99) THz, the second band gaps (143–190) THz, the third band gaps (240–262) THz, and fourth band gaps (321–340) THz. In the same way, the width of the PBGs are (58–94) THz for first, (134–182) THz for the second, (224–254) THz for the third, and (310–318) THz for the fourth for the  $AgInSe_2$ , respectively. For  $CuGaS_2$ , the first TE band gaps appeared to be between the first and second bands in the frequency ranges of (63–100) THz, the second band gaps (145–192) THz, the third band gaps (242–265) THz, and fourth band gaps (325–342) THz. Finally, the width of the PBGs are



**Figure 2** TE Transmittance spectrum of  $CuGaS_2$  based Conventional and Fibonacci Photonic crystal structures of 5th (a) and 10th generations.

**Table 2** Variation of the full band gap size with the filling factor for TE modes of anisotropic  $A^{III}B^{III}C^{VI}_2$  based layers in an air background.

material	filling factor	TE1		TE2	
		band gap (THz)	gap size (%)	band gap (THz)	gap size (%)
$AgGaS_2$	0.1	(107–148)	16.35	(229–294)	12.55
	0.3	(77–134)	27.11	–	–
	0.6	(64–93)	18.18	(140–183)	13.09
	0.9	(61–68)	4.82	(124–136)	4.35
$AgGaSe_2$	0.1	(101–148)	18.99	(221–293)	13.92
	0.3	(71–131)	29.49	(199–206)	1.62
	0.6	(59–87)	18.94	(130–172)	13.94
	0.9	(57–62)	4.73	(114–125)	4.60
$AgInSe_2$	0.1	(95–149)	22.13	(215–291)	15.02
	0.3	(67–127)	30.93	(187–203)	4.10
	0.6	(56–82)	18.84	(121–162)	14.48
	0.9	(53–59)	5.35	(107–117)	4.46
$CuGaS_2$	0.1	(101–189)	30.34	(221–293)	14.00
	0.3	(72–131)	29.06	(199–208)	2.21
	0.6	(61–88)	18.12	(132–173)	13.44
	0.9	(58–64)	4.91	(117–127)	4.09
$CuInS_2$	0.1	(95–149)	22.13	(215–291)	15.01
	0.3	(67–127)	30.92	(187–203)	4.10
	0.6	(56–82)	18.84	(122–162)	14.08
	0.9	(54–59)	4.42	(108–117)	4.00

(58–94) THz for first, (134–182) THz for the second, (224–254) THz for the third, and (311–319) THz for the fourth for the  $CuInS_2$ , respectively. 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 from Fig. 1(a, b, c, d, and e), transmittance is zero in this range of frequencies where the refractive index of the structure is positive and the spectral width of the gaps is invariant with the change in the transmittance (Table 2).

Variation of the full band gap size with a filling factor for the TE modes of  $A^I B^{III} C^{VI}_2$  based CPhc are given in Table 2. The variation of the band gap sizes (%) as a function of filling factor changes between 4 and 31 for all types of crystals. The largest gap size is approximately 31% when the filling factor is as high as 0.3, but it decreases when the filling factor continues to increase. On the other hand, the second band gap size do not change too much according to the filling factor.

We also calculate the spectral properties for  $n$ -th ( $n = 5$  and 10) generation Fibonacci-type quasi-periodic layered structures consisting of  $A^I B^{III} C^{VI}_2$  compounds. The Fig. 2 show the transmittance spectra of  $CuGaS_2$  (as an example) based both Conventional Phc and Fibonacci Phc of  $n$ -th ( $n = 5$  and 10) generations for the TE-polarized incident electromagnetic wave. The obtained transmission spectra show that the optical properties of the structure depend on the parity of  $n$ . The two spectra (Fig. 2) present bands of oscillations, one of which centered always in  $\omega = 170$  THz for  $CuGaS_2$ . These bands narrow and the number of oscillations increase as  $n$  increases. On the other hand, the positions of the minima in the transmission spectrum correlate with the gaps obtained in the calculation. A transmission spectrum of a simple two generation-layers (also  $n = 5$  and 10) 1D  $A^I B^{III} C^{VI}_2$  based CPC is compared in Fig. 2 with an same generation layers 1D  $A^I B^{III} C^{VI}_2$  based FPC.

One full period in the spectrum is presented which corresponds to the frequency range between 130 and 195 THz. Although there is still a gap in the transmission spectrum of the Fibonacci structure around (170 THz), the spectrum modified significantly. Notably, the total number of transmission peaks in both cases was equal to the total number of elementary layers in the structure. This is the general property of multilayer structures. In addition, the spectral regularities inherent in Fibonacci structures have also been derived in analytical form based on the transfer matrix approach. Fibonacci structures feature a transmission band in the center that first splits into two and then into three subbands (Fig. 2). This central triplet is indicative for the Cantor triadic set and for higher generations, definite self-similar and scaling features develop that are inherent in fractals. Different portions of transmission spectra for the

same high-order generation of Fibonacci structures exhibit a similar spectral shape that becomes apparent when using the “exciton in quantum dot” lowest state energy expansion [1]. The transmission spectra of Fibonacci structures also show scalability which means that the spectra of different generations have a similar shape when the frequency axis is properly scaled. Notably, the transmission spectra of generic Fibonacci structures exhibit perfect transmission bands.

**4 Conclusions** The photonic band structures and transmission properties of the 1D  $A^I B^{III} C^{VI}_2$  based conventional PCs and Fibonacci PCs consisting of dielectric layers immersed in air were studied. The numerical results of the variation of the full band gap with a changing filling factor show that the largest gap size occurs when the filling factors are 0.3 for 1D. We have also investigated the spectral properties for  $n$ -th ( $n = 5$  and 10) generations Fibonacci-type quasi-periodic layered structures consisting of  $A^I B^{III} C^{VI}_2$  compounds. The obtained transmission spectra show that the optical properties of the structure depend on the parity of  $n$ .

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