Physica Status Solidi C: Current Topics in Solid State Physics

# AIBIIICVI2 (A=Cu, Ag; B=Ga, In; C=S, Se, Te) Based Photonic Crystal Superlattices: Optical Properties

--Manuscript Draft--

| | |
|---|---|
| **Manuscript Number:** | pssc.201600156R3 |
| **Full Title:** | AIBIIICVI2 (A=Cu, Ag; B=Ga, In; C=S, Se, Te) Based Photonic Crystal Superlattices: Optical Properties |
| **Article Type:** | Feature Article |
| **Section/Category:** | ICTMC-20 |
| **Keywords:** | Fibonacci sequence, Photonic Crystal, FDTD, AIBIIICVI2. |
| **Corresponding Author:** | Amirullah Mamedov, Hab. Dr. Sciences<br>Bilkent Universitesi<br>Ankara, Ankara TURKEY |
| **Additional Information:** | |
| **Question** | **Response** |
| Please submit a plain text version of your cover letter here.<br><br>Please note, if you are submitting a revision of your manuscript, there is an opportunity for you to provide your responses to the reviewers later; please do not add them to the cover letter. | Dear Sir<br><br>I send our manuscript entitled “AIBIIICVI2 (A=Cu, Ag; B=Ga, In; C=S, Se, Te) Based Photonic Crystal Superlattices: Optical Properties” for peer review and publication in Physica Status Solidi C. Current Topics in Solid State Physics.<br><br>Thank You in advance,<br><br>I hope to hear You as soon as possible.<br><br>Sincerely Yours<br><br>Prof. Dr. Amirullah M.Mamedov,<br>Bilkent University, NANOTAM |
| **Corresponding Author Secondary Information:** | |
| **Corresponding Author's Institution:** | Bilkent Universitesi |
| **Corresponding Author's Secondary Institution:** | |
| **First Author:** | Amirullah Mamedov, Hab. Dr. Sciences |
| **First Author Secondary Information:** | |
| **Order of Authors:** | Amirullah Mamedov, Hab. Dr. Sciences |
| | Sevket Simsek, Dr. |
| | Selami Palaz, Dr. |
| | Chingiz Akhundov |
| | Ekmel Ozbay |
| **Order of Authors Secondary Information:** | |
| **Manuscript Region of Origin:** | TURKEY |
| **Abstract:** | In this study, we present an investigation of the optical properties and band structures for the photonic structures based on AI-BIIICVI2 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 the so-lution of Maxwell's equations. |

pss-Header will be provided by the publisher



# $A^{I}B^{III}C^{VI}_2$ (A=Cu, Ag; B=Ga, In; C=S, Se, Te) Based Photonic Crystal Superlattices: Optical Properties

**Sevket Simsek[1], Selami Palaz[2], Chingiz Akhundov[3], Amirullah M. Mamedov [*,3,4] , and Ekmel Ozbay[4]**

[1] Hakkari University, Faculty of Engineering, Department of Material Science and Engineering, 3000, Hakkari, Turkey
[2] Harran University, Faculty of Science and Letters, Department of Physics, 63000, Sanliurfa, Turkey
[3] Baku State University, International Scientific Center, Baku, Azerbaijan
[4] Bilkent University, Nanotechnology Research Center, 06800, Ankara, Turkey

Received ZZZ, revised ZZZ, accepted ZZZ
Published online ZZZ (Dates will be provided by the publisher.)

**Keywords** Fibonacci sequence, Photonic Crystal, FDTD, $A^{I}B^{III}C^{VI}_2$.

* Corresponding author: e-mail mamedov@bilkent.edu.tr, Tel.: +90 312 290 1966, Fax: +90 312 266 4042

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.



**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 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 (A=Ag, Cu; B=In, Ga, Al; C=Se, Te, S) are very useful nonlinear optical materials in a wide optical range from 0.7 to 20μm. [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 paper, we study the one dimensional (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…, 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, …}. 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 $A^IB^{III}C^{VI}_2$ (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 $a = (d_A + d_B) = 1\ \mu m$. 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 $A^IB^{III}C^{VI}_2$ materials are taken from Ref. [7,8] and are given in Table 1.The refractive index of the background dielectric medium is assumed as air ($n_{air}$=1.0).

**Table 1** The refractive index of $A^IB^{III}C^{VI}_2$ materials.

| Material | $n_x$ (=$n_o$) | $n_y$ (=$n_o$) | $n_z$ (=$n_e$) | *λ (μm) | Ref. |
|---|---|---|---|---|---|
| $AgGaS_2$ | 2.408 | 2.408 | 2.355 | 0.6 | [7] |
| $AgGaSe_2$ | 2.617 | 2.617 | 2.586 | 0.6 | [7] |
| $AgInSe_2$ | 2.7971 | 2.7971 | 2.8453 | 1.10 | [7] |
| $CuGaS_2$ | 2.5681 | 2.5681 | 2.5630 | 0.90 | [8] |
| $CuInS_2$ | 2.7907 | 2.7907 | 2.7713 | 0.90 | [8] |

*λ = wavelength, at which the refractive index is measured

**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,

$\varepsilon(\boldsymbol{r})$ is the space dependent dielectric function

$c$ is the speed of light in vacuum.

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

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 $A^IB^{III}C^{VI}_2$ 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 $A^IB^{III}C^{VI}_2$ 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 (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).

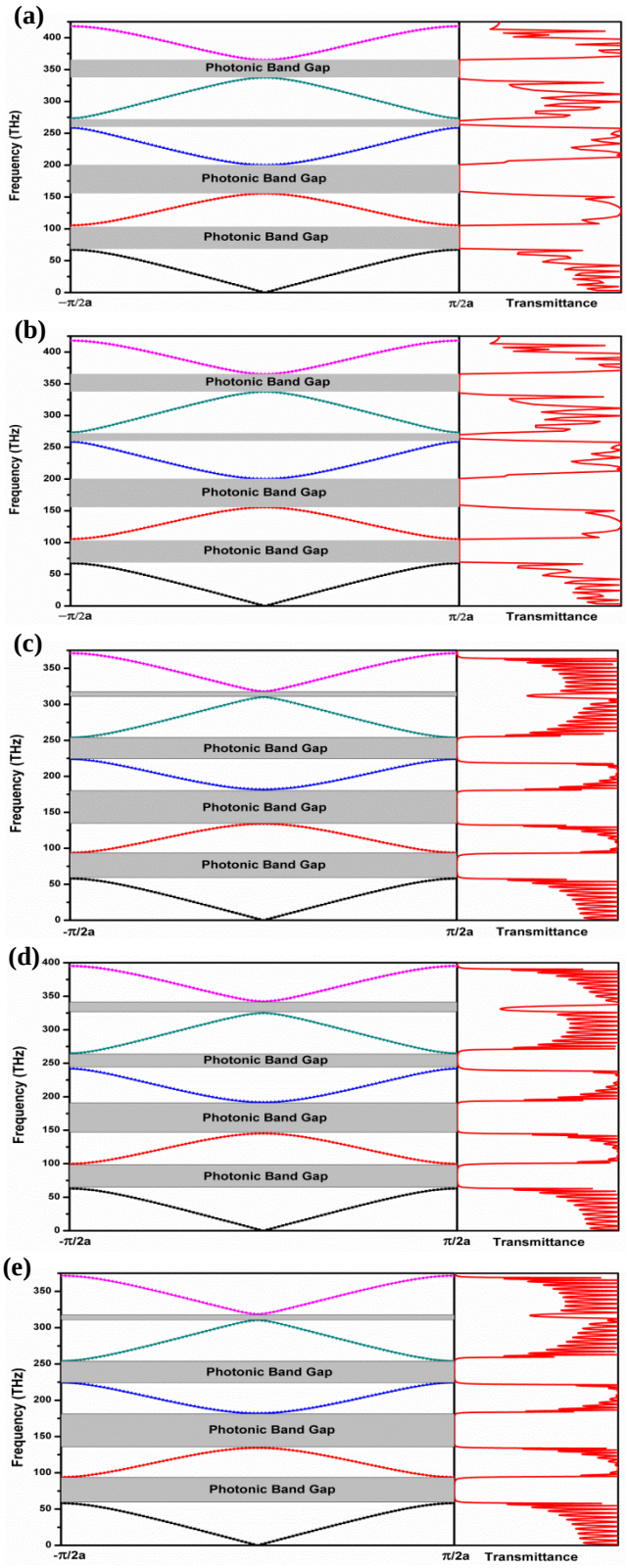


**Figure 1** TE Band structure and transmittance spectra of $A^{I}B^{III}C^{VI}_2$ based CPhc in 1D. $AgGaS_2$ (a), $AgGaSe_2$ (b), $AgInSe_2$ (c), $CuGaS_2$ (d) and $CuInS_2$ (e).

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 approx. 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 n=10) generation Fibonacci-type quasi-periodic layered structures consisting of $A^{I}B^{III}C^{VI}_2$ compounds. The Figs. 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 ω=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.

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

| | | TE1 | | TE2 | |
|---|---|---|---|---|---|
| Material | Filling Factor | 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 |

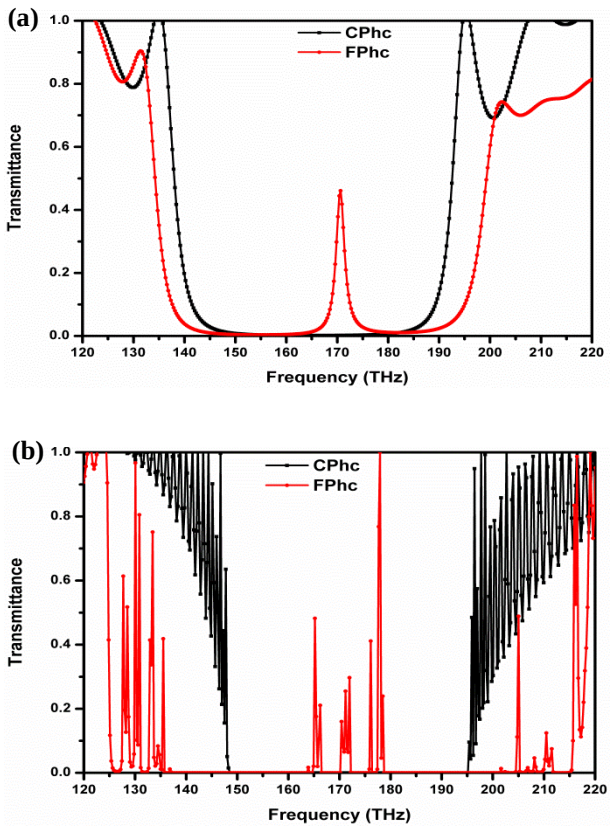


**Figure 2** TE Transmittance spectrum of $CuGaS_2$ based Conventional and Fibonacci Photonic crystal structures of 5th (a) and (b) 10th generations.

**4 Conclusion** 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 n=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*.

**Acknowledgements** This work is supported by the projects DPT-HAMIT, DPT-FOTON, and NATO-SET-193 as well as TUBITAK under Project Nos. 113E331, 109A015, and 109E301. One of the authors (Ekmel Ozbay) also acknowledges partial support from the Turkish Academy of Sciences.

## References

[1] S. V. Gaponenko, Introduction to Nanophotonics, (Cambridge University Press N.Y, 2010), p. 465.
[2] H. Rahimi, A. Namdar, S. R. Entezar, H. Tajalli, Progress In Electromagnetics Research **102**, 15 (2010).
[3] L. D. Negro, C. J. Oton, Z. Gaburro, L. Pavesi, P. Johnson, A. Lagendijk, R. Righini, M. Colossi, D. S. Wiersma, Phys. Rev. Lett. **90**, 055501 (2003).
[4] S. Chen, X. G. Gong, and S. H. Wei, Phys. Rev. B **75**, 205209 (2007).
[5] M. T. Whittakera, T. E. Stengera, D. G. Krausea, D. H. Matthiesen, Journal of Crystal Growth **310**, 1904 (2008).
[6] S. G. Gupta, Optoelectronic Devices and Systems (second ed.), (PHI Learning, Prentice-Hall Pvt. Ltd, 2015)
[7] William J .Tropf, Michael E. Thomas, and Terry J. Harris, Optical and Physical Properties of Materials, Chapter 33 1-100.
[8] E. D. Palik, Handbook of Optical Constants of Solids, (Academic Press, New York, USA, 1998), p. 337.
[9] OptiFDTD 10, http://www.optiwave.com/.
[10] A. Taflove and S. C. Hagness, Computational Electrodynamics: The Finite-Difference Time-Domain Method 2nd ed., (MA: Artech House Publishers, Boston, 2000), p. 997.