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Complete photonic band gaps in $\text{Sn}_2\text{P}_2\text{X}_6$ ($\text{X} = \text{S}, \text{Se}$) supercell photonic crystals

Sevket Simsek^a, Selami Palaz^b, Husnu Koc^c, Amirullah M. Mamedov^{d,e}, and Ekmel Ozbay^d

^aDepartment of Material Science and Engineering, Hakkari University, Hakkari, Turkey; ^bDepartment of Physics, Faculty of Science and Letters, Harran University, Sanliurfa, Turkey; ^cDepartment of Physics, Faculty of Science and Letters, Siirt University, Siirt, Turkey; ^dNanotechnology Research Center, Bilkent University, Ankara, Turkey; ^eInternational Scientific Center, Baku State University, Baku, Azerbaijan

ABSTRACT

In this work, we present an investigation of the optical properties and band structures for the photonic crystal structures (PCs) based on $\text{Sn}_2\text{P}_2\text{X}_6$: $\text{X} = \text{S}, \text{Se}$) with Fibonacci superlattices. The optical properties of PCs 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 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.

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1. Introduction

It is well known that photonic crystal (PC) based superlattices can play an essential role in the controlling of the optical processes in various devices of optoelectronics [1]. Therefore, great attention is paid to the investigation of the physical properties of PC based superlattices. The PC based superlattices of various types are considered, namely, as strictly periodic, disordered, lattices with defects, etc. The structures intermediate between the periodic and disordered structures or quasi-periodic lattices – the Fibonacci and Thue-Morse superlattices – occupy a special place among the superlattices. On the other hand, one of the topics of interest in the optics of PC is the possibility to tailor the emittance/absorptance by changing the distribution of electromagnetic modes. Emittance tailoring by conventional PCs was investigated in [2, 3]. One of the structures that may be used in emittance tailoring is quasiperiodic multilayers, such as Fibonacci superlattices [4]. Due to their structural self-similarity, these show regularities in their transmission/reflection spectra. The strong resonances in the spectral dependences of fractal multilayers can localize light very effectively [1, 4]. 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 [1, 4]. On the other hand, a one-dimensional Schrödinger equation has been examined with a stepwise quasiperiodic potential whose value is equal to either of the two fixed values sequentially in accordance with the Fibonacci set [1]. For such a potential, an electron was found to have a “critical wave function” with strong spatial fluctuations. This type of wave function correlates with the properties of the energy spectrum. 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 the present paper, we investigated the energy spectrum and optical properties in the Fibonacci-type photonic band gap structures consisting of ferroelectric material ($\text{Sn}_2\text{P}_2\text{X}_6$; $\text{X} = \text{S}, \text{Se}$) in detail by using the finite-difference time-domain (FDTD) method and the plane wave expansion method (PWE). The choice of the $\text{Sn}_2\text{P}_2\text{X}_6$ crystals as the active media for our investigation was associated with their unusual optical and electronic properties. It is well known that $\text{Sn}_2\text{P}_2\text{X}_6$ are the ferroelectric materials and their properties are very sensitive to external influences (temperature, electric field, stress, and light) [5]. Therefore, $\text{Sn}_2\text{P}_2\text{X}_6$ based Fibonacci photonic crystal may be used as efficiency material for photonic devices.

2. Computational details and model

All calculations have been performed using on the finite-difference time-domain (FDTD) [1] method for the transmission spectra as well as plane wave expansion method (PWE) for the photonic band structure in the OptiFDTD package [2]. The FDTD algorithm divides space and time in a regular grid for solving Maxwell's equations depending on the time, and solves the electric and magnetic fields by rating depending on space and time. This procedure is known as Yee grid discretization. Fields in these grids can be classified as Transverse Magnetic (TM) and Transverse Electric (TE) polarization. Perfect matched layers (PMLs) can be used in the determination of the boundary conditions [3]. In the transmission spectra calculations, we have used Perfect Magnetic Conductor (PMC) and Anisotropic Perfectly Matched Layer (APMLs) boundary conditions at the x- and z-directions, respectively.

The photonic band structures of the proposed PCs are based on 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, $\varepsilon(\mathbf{r})$ and c are the space dependent dielectric function and the speed of light in vacuum, respectively. $\mathbf{H}(\mathbf{r})$ 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

Figure 1. Illustration of (a) the Conventional lattice and (b) the Fibonacci lattice.

terms of the electric field. If the structure has infinite periodicity, the Bloch theorem can be given in the following form:

$$\mathbf{H}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{h}_k(\mathbf{r}) \quad (2)$$

Where

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

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

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

The photonic band structure can be obtained by solving these equations in the irreducible Brillouin zone. A 1D quasi-periodic 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 $S_0 = \{B\}$, $S_1 = \{A\}$, $S_2 = \{BA\}$, $S_3 = \{ABA\}$, $S_4 = \{BAABA\}$ and soon, where S_j is a structure obtained after j iterations of the generation rule [4]. Here, A and B represent 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 $\text{Sn}_2\text{P}_2\text{S}_6$ and $\text{Sn}_2\text{P}_2\text{Se}_6$ for A material and air for B material. In Figure 1 (a) and (b), we schematically show the geometry of Conventional Photonic Crystal (CPCs) and Fibonacci Photonic Crystal (FPCs). The thickness of the considered layers of A and B is $d_A = 0.5a$ and $d_B = 0.5a$, respectively. The lattice constant is $a = 1 \mu\text{m}$. 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. $f = d_1/(d_1+d_2)$. The filling fraction is set to 0.5. The refractive index contrasts of $\text{Sn}_2\text{P}_2\text{S}_6$ and $\text{Sn}_2\text{P}_2\text{Se}_6$ are taken as 2.10 and 2.76, respectively. The refractive index of the background dielectric medium is assumed as air ($n_{\text{air}} = 1.0$).

3. Results and discussion

We calculate the spectral properties in the n -th order ($n = 5, 6, 7, 8$) Fibonacci-type quasiperiodic layered structures consisting of compounds. The band structures of 1D $\text{Sn}_2\text{P}_2\text{X}_6$ based PCs have been calculated in high-symmetry directions in the first

Figure 2. TE Band structure and transmission spectra of (a) $\text{Sn}_2\text{P}_2\text{S}_6$ and (b) $\text{Sn}_2\text{P}_2\text{Se}_6$ based 1D CPhC

Brillouin zone. The band structures with transmittance spectra for $\text{Sn}_2\text{P}_2\text{X}_6$ based photonic crystals are shown in Figure 2. We can see that there exist four fundamental stop band gaps (SBG) for $\text{Sn}_2\text{P}_2\text{S}_6$ and five SBG for $\text{Sn}_2\text{P}_2\text{Se}_6$. The width of the fundamental SBG are $[0.25-0.38 \text{ (} 0.19-0.32 \text{)}] (\omega a/2\pi c)$ for the 1st SBG, $[0.58-0.71(0.45-0.61)] (\omega a/2\pi c)$ for 2nd SBG, $[0 (0.76-0.85)] (\omega a/2\pi c)$ for 3rd SBG and $[1.23-1.35 (1.04-1.09)] (\omega a/2\pi c)$ for 4th SBG of $\text{Sn}_2\text{P}_2\text{S}_6$ and $\text{Sn}_2\text{P}_2\text{Se}_6$ based PCs, respectively. When the frequency of an incident wave drops in these SBGs, the electromagnetic wave will be reflected completely from the PC. It can be seen in Figure 2 that the transmittance is zero in these range of frequencies. All SBGs exist in the frequencies where the effective refractive index of the structures is positive and the spectral width of the gaps are invariant with the change in the transmittance (Tables 1 and 2).

Table 1. Variation of the full band gap size for TE modes with a filling factor for the $\text{Sn}_2\text{P}_2\text{S}_6$ based layers in air background.

Filling Factor	TE1		TE2		TE3		TE4	
	Band Gap ($\omega a/2\pi c$)	Gap Size (%)	Band Gap ($\omega a/2\pi c$)	Gap Size (%)	Band Gap ($\omega a/2\pi c$)	Gap Size (%)	Band Gap ($\omega a/2\pi c$)	Gap Size (%)
0.1	(0.38-0.49)	25.28	(0.80-0.99)	21.22	(1.26-1.46)	14.70	(1.74-1.91)	9.31
0.2	(0.32-0.48)	40.00	(0.74-0.91)	20.60	–	–	(1.56-1.72)	9.75
0.3	(0.29-0.46)	45.33	(0.73-0.77)	5.33	(1.05-1.21)	14.16	(1.47-1.55)	5.29
0.4	(0.26-0.42)	47.05	(0.66-0.73)	10.07	(0.98-1.10)	11.53	(1.33-1.46)	9.31
0.5	(0.25-0.38)	41.26	(0.58-0.71)	20.15	–	–	(1.23-1.35)	9.30
0.6	(0.24-0.34)	34.48	(0.53-0.67)	23.33	(0.86-0.96)	10.99	–	–
0.7	(0.24-0.31)	25.45	(0.50-0.61)	19.82	(0.78-0.91)	15.38	(1.08-1.19)	9.69
0.8	(0.23-0.28)	19.60	(0.48-0.56)	15.38	(0.74-0.84)	12.65	(1.00-1.12)	11.32
0.9	(0.23-0.25)	8.33	(0.47-0.51)	8.16	(0.71-0.77)	8.10	(0.96-1.03)	7.03

Table 2. Variation of the full band gap size for TE modes with a filling factor for $\text{Sn}_2\text{P}_2\text{Se}_6$ based layers in air background.

Filling Factor	TE1		TE2		TE3		TE4	
	Band Gap ($\omega a/2\pi c$)	Gap Size (%)	Band Gap ($\omega a/2\pi c$)	Gap Size (%)	Band Gap ($\omega a/2\pi c$)	Gap Size (%)	Band Gap ($\omega a/2\pi c$)	Gap Size (%)
0.1	(0.32-0.49)	41.97	(0.72-0.98)	30.58	(1.19-1.42)	17.62	(1.68-1.78)	5.78
0.2	(0.26-0.47)	57.53	(0.68-0.82)	18.66	(1.05-1.17)	10.81	(1.38-1.60)	14.76
0.3	(0.22-0.43)	64.61	(0.64-0.68)	6.06	(0.89-1.08)	19.28	(1.28-1.36)	6.06
0.4	(0.20-0.37)	59.64	(0.52-0.66)	23.72	(0.86-0.91)	5.64	(1.09-1.26)	14.46
0.5	(0.19-0.32)	50.98	(0.45-0.61)	30.18	(0.76-0.85)	11.18	(1.04-1.09)	3.77
0.6	(0.18-0.27)	40.00	(0.41-0.55)	29.16	(0.67-0.81)	18.91	(0.94-1.03)	9.14
0.7	(0.18-0.24)	28.57	(0.38-0.49)	25.28	(0.60-0.73)	19.54	(0.84-0.97)	14.36
0.8	(0.18-0.22)	20.00	(0.37-0.44)	17.28	(0.56-0.66)	16.39	(0.77-0.88)	13.33
0.9	(0.18-0.20)	5.40	(0.36-0.40)	10.52	(0.55-0.60)	8.69	(0.73-0.79)	7.89

The numerical results of the variation of a full SBG with a changing filling factor from 0.1 to 0.9 are given in Tables 1 and 2.

The variation of the full band gap sizes with a filling factor for TE modes show that the first TE band gaps of both materials are the most affected by the filling factor. The first and second TE band gaps for $\text{Sn}_2\text{P}_2\text{X}_6$ display opposite characteristics when the filling factor is 0.3. The largest gaps size for the first TE band emerges, when the filling factor is 0.3. Then, they decrease when the filling factor continues to increase. On the other hand, the second TE band gaps reaches the minimum value when the filling factor is 0.3. Moreover, the first and second TE band gap sizes of both materials show similar characteristics, respectively.

The position of transmittance spectra of $\text{Sn}_2\text{P}_2\text{X}_6$ based both normal PCs and FPCs from 8 to 55 layers for the TE mode show the good correlation with the gaps obtained in the calculation. A transmission spectrum of a n layers (from 8 to 55 layers) 1D $\text{Sn}_2\text{P}_2\text{X}_6$ based CPC is compared with the same layers 1D $\text{Sn}_2\text{P}_2\text{X}_6$ based FPC.

4. Conclusions

In the present paper, the photonic band structures and transmission properties of the 1D $\text{Sn}_2\text{P}_2\text{X}_6$ PCs consisting of dielectric layers immersed in air were studied for the first time. We have investigated the transmittance spectra of $\text{Sn}_2\text{P}_2\text{X}_6$ based on normal PCs and FPCs from 8 to 55 layers. The results show that the number of the repetition

period also has a great influence on the average transmittance of the pass band of the both normal PCs and FPCs.

References

- [1] A. Taflove, and S. C. Hagness, *Computational Electrodynamics: The Finite-Difference Time-Domain Method* (Boston, Artech House Publisher 2000).
- [2] <http://www.optiwave.com/>
- [3] J. P. Berenger, A perfectly matched layer for the absorption of electromagnetic waves, *J. Comput. Phys.* **114** (2), 185 (1994). DOI: [10.1006/jcph.1994.1159](https://doi.org/10.1006/jcph.1994.1159).
- [4] S. V. Gaponenko, *Introduction to Nanophotonics* (New York, Cambridge University Press 2010).
- [5] M. Zhao *et al.*, Enhancing visible light absorption for ferroelectric Sn₂P₂S₆ by Se anion substitution, *J. Phys. Chem. C.* **122** (44), 25565 (2018). DOI: [10.1021/acs.jpcc.8b08402](https://doi.org/10.1021/acs.jpcc.8b08402).