

Influence of defect layer of ZnS/air on one dimensional photonic crystal structure of gallium phosphide-crown glass using numerical FDTD

K. PRATIBHA¹, MANISH SINGH¹, S. SONI¹, TANNU GARG¹, VINITA TULI², S. GAURAV^{1,*}, S. SHANKAR^{2,*}

¹Department of Applied Physics, AIAS, Amity University, Noida, U.P.-201303, India

²Experimental Research Laboratory, Department of Physics, ARSD College, University of Delhi, Dhaula Kuan, New Delhi-110021, India

The reflectance characteristics of defect modes in a one-dimensional photonic crystal structure are studied theoretically using Numerical FDTD software. Photonic crystal (PC) consisting of alternating layers of Gallium Phosphide and crown glass are modelled along with dielectric defect layers of ZnS and Air. The reflectance spectra of PC have been studied without defect layer and for different thicknesses of defect layer by simulation. The reflectance spectrum of PC without defect displayed 100% reflectivity in the near-IR region owing to its high refractive index and indirect band gap. The introduction of defect layer in PC modified the spectra by displaying one or more peaks due to modification in periodicity of PC. The spectra exhibited that variation in thickness of a defect layer (ZnS) impacted the tunability of photonic band gap without altering other characteristics in conventional PCs. Furthermore, the impact of dielectric defect layer (ZnS) is also compared with layer of Air and impact of Air is found to be prominent than that of ZnS. The origin of double defect modes with larger thickness are validated with electromagnetic theory. These results suggest that photonic crystal of Gallium Phosphide and Crown Glass with dielectric defect layer of ZnS/Air has potential for tunable tunnelling/transmission modes for suitable photonic, frequency filtering, optoelectronic and optomechanical applications.

(Received August 18, 2021; accepted June 7, 2022)

Keywords: Photonic crystal structure, Defect modes, Tunnelling, Refractive index

1. Introduction

The interaction of electromagnetic wave with matter/particles forms the premise of the basic phenomena such as emission, absorption, transmission, and reflection. The potential to manipulate these interactions opens up opportunities suitable for novel technological applications such as optoelectronic sources, cells, detectors and optical data processing. [1]. In this regard, over the last three decades, photonic crystals have attracted researchers round the globe owing to their potential ability of controlling and manipulating electromagnetic light waves by the periodic system [2,3]. Photonic crystals (PC) are fascinating optical materials characterized as natural or artificial assemblies and display regular variation of refractive index [4]. These materials have constant variation of dielectric constant in either one or two or all the orthogonal directions [5]. These capable systems exhibit robust behaviour in manipulating the light as analogous to electron control in electronic devices [6,7]. PCs are observed to be promising in the applications of detectors, photovoltaic cells and Tera Hertz devices due to minimum loss, low dispersion and transparency in the THz band or near-IR region [8]. PCs are capable of trapping light by changing its parameters [9,10]. These crystals use dielectric materials in periodic fashion having band gap and create allowed/forbidden bands for incoming light [2,11]. The studies on PCs are important for photonic device applications in field of optics,

material science and solid-state physics [4,11]. Like a semiconductor band gap which does not support electrons, a photonic band gap (PBG) does not support photons [12]. When an electromagnetic wave is incident on the PC, some electromagnetic fields propagate through the PC, but others cannot due to the forbidden photonic bandgap [5]. This bandgap arises on account of multiple Bragg scattering of the incident light. The parameters of this forbidden bandgap can be tailored by periodicity of PC and parameters of medium [13]. These crystals use dielectric materials like Si, Ge, InP, and GaAs to fabricate them because they are comparatively lossless which enable the light wave to propagate through them without any attenuation and make them useful in making optic-electrical devices [11,14,15].

The manifestation of defect modes inside the PBG is a fascinating subject of research. With the insertion of defect layer inside PC, localization of photons is possible within the forbidden bandgap. By varying the refractive index of the defect medium, the position of defect mode can be tailored because of robust confinement of field inside the defect layer. This purview of defected PC could be employed in sensing of refractive index [5]. The creation of a defect by adding an impurity or removing any layer pulls a light mode into the PBG which makes transmission at that particular wavelength possible and can be useful in designing optical fibres [16,17]. These defect modes are created by breaking translational symmetry in photonic crystal [18]. The defect material acts as cavity and generates

tunnelling modes. The presence of these tunnelling modes can be identified from occurrence of sharp peak in transmission or reflection spectra [17,19]. Dielectric defect layers are most preferred for PC crystals as they provide additional tuning with temperature and width [20]. This tuning characteristic renders defect mode of PC in optical communications. Among these dielectric materials, Zinc sulphide (ZnS) is commonly used as defect because of its wide gap and low absorption, direct transition semiconductor and intermediate refractive index [21]. Additionally, ZnS has low dielectric value in near-IR region. Therefore, it has been used for antireflection coating for heterojunction solar cells [21].

Presently, PCs are modelled by calculating transmission and reflection coefficient parameters [22,23]. Some of the numerical estimation techniques of these parameters include plane wave expansion method, the generalized Rayleigh identity method, and matrix method and finite-difference time-domain method [24]. All these methods have their advantages and disadvantages in obtaining characteristics of defects modes of one-dimensional PC. Among these, the finite-difference time domain (FDTD) method is the most appropriate method for obtaining electromagnetic properties within a single run with better efficiency [24,25]. FDTD is basically a technique which solves Maxwell equation in the time domain using finite difference approximations. This technique can be used to visualise how the waves are interacting with the designed structure [7,26]. Lumerical software employs numerical estimation technique like finite element method for solving the equations governing on electromagnetic wave propagation inside PC like Maxwell's equations, etc. and computes as well as presents various reflectance and transmittance curves [27].

PCs depend on refractive index variation and thus possessing high refractive index is a desirable material characteristic. In this work we intend to study the PC consisting of gallium phosphide (GaP) having high refractive index of 3.05 and an indirect bandgap of 2.26 eV [28]. GaP is therefore transparent largely in visible region [29]. GaP displays high dispersion of index in the Near-IR region (0.7-5 μm) owing to its lone absorption peak [30]. In order to minimise this optical loss of GaP, it can be modelled with materials of minimum dispersion. In this regard, Crown Glass (CG) stands out as a potential material having low dispersion in Near-IR region [31,32]. Combining GaP with CG in a photonic crystal could result in minimum dispersion in the Near-IR region. Though there has been work on photonic crystal based on GaP [28,33] and crown glass [31,32] respectively. However, investigations on GaP modelled with CG hasn't been reported yet. This work aims to investigate the behaviour of PC of multilayer of GaP and CG. In this work, the Lumerical FDTD software has been employed to investigate the optical properties of defect modes of ZnS and air within reflection band of the one-dimensional photonic crystal of GaP and crown glass.

2. Modelling of photonic crystal structure

The one-dimensional Photonic Crystal (PC) comprising of alternating multilayer of material A (Crown Glass) and material B (Gallium Phosphide) with refractive index 1.5 and 3.5 respectively is modelled in the form $(AB)^{10}$. The defect modes are incorporated in the PC by inserting the dielectric defect layer D (ZnS/Air) at the centre of PC in the form $(AB)^5D(AB)^5$. Figs. 1-3, represent the modelled PC without defect, PC with ZnS as defect layer and PC with Air as defect layer respectively. The layer of material A, material B and defect layer D are coloured as reddish brown, yellow and sky-blue colour respectively. The substrate material (flint glass) with refractive index 1.5 used with PC is coloured in pink. The blue line with arrows is the source of electromagnetic wave from air to PC and the greenish-yellow line represents the detector for measurement of reflectance. The orange-colored box in which all the structures are designed is the simulation domain.

The working layout of the numerical FDTD is a step-by-step process. These steps were followed to design required structure of PC:

- **Creating physical structures:** The structure was broken down into small units as the structure on the numerical FDTD was made step by step. The (n,k) model was used when a refractive index is added at a single frequency and that frequency is the central frequency of the source.
- **Set simulation parameters:** The FDTD simulation domain set the boundaries for the region where simulation was going to be performed. The simulation region also affected the time frame for which simulation was going to be performed i.e. smaller the simulation region, the lesser time it took to run the simulation. The boundary condition of the simulation domain play an important role in running the simulation.
- **Define sources:** The next necessary element required to be added in the simulation domain is the source which injected light into the designed structure. There are various types of sources available namely plane wave, Gaussian, mode source, dipole and TFSF source which can be used depending upon the need of the user.
- **Define monitors:** Monitors are useful for monitoring the light wave propagation into the structure of interest. There are different types of monitors namely frequency domain field profile monitor, index monitor, time monitor, movie monitor, mode expansion monitor, frequency domain field and power monitor which can be used depending upon the type of effect which is to be visualized.
- **Check simulation:** After the desired structure was designed, the changes are required to be saved with the required file name. Then the mesh size was needed to be calculated and the memory requirements were needed to be checked. The mesh size was needed to be recalculated each time before running a simulation.
- **Run simulation:** Then clicked on the run the simulation button.

- Analyze the results: The results of the simulation was visualized by the right clicking on the monitor placed on the left side of the window in a separate column.

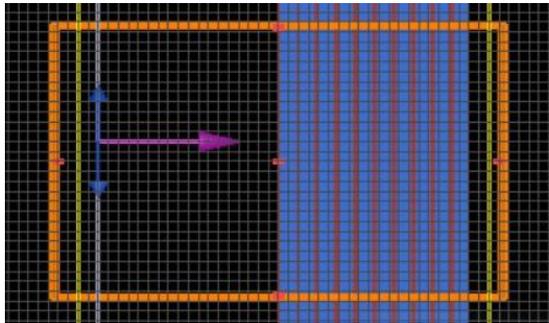
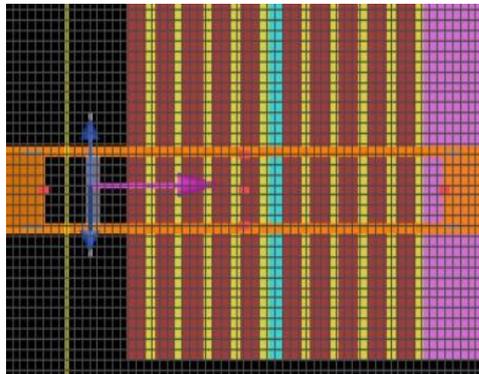
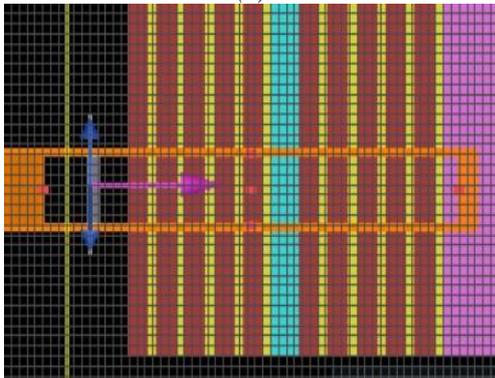


Fig. 1. Modelled Photonic crystal of Gallium Phosphide(A) and Crown Glass(B) as $(AB)^{10}$ without defect and $a=0.042$ microns and $b=0.15$ microns (color online)

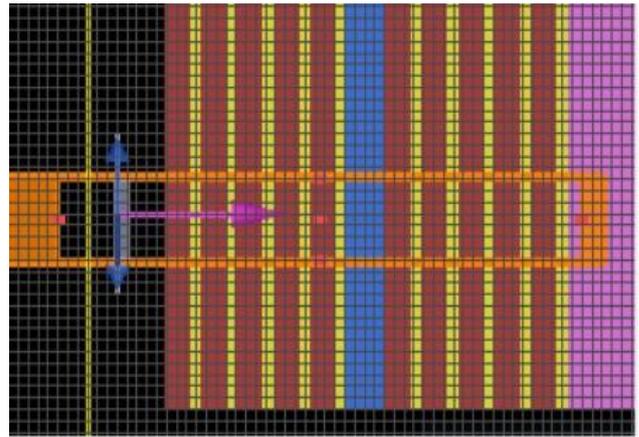


(a)

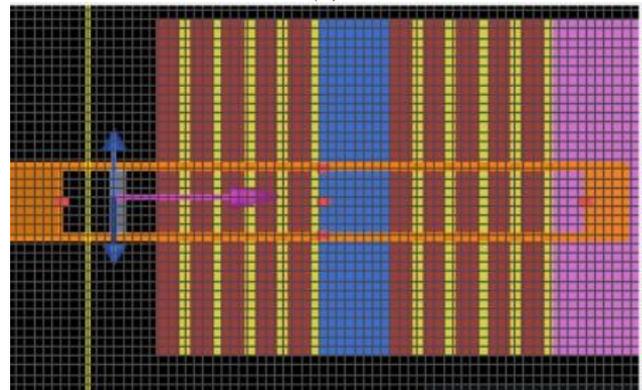


(b)

Fig. 2. Photonic crystal of Gallium Phosphide(A) and Crown Glass(B) of the form $(AB)^5D(AB)^5$ with ZnS (D) as defect layer with thickness (a) 0.1685 and (b) 0.337 microns (color online)



(a)



(b)

Fig. 3. Photonic crystal of Gallium Phosphide(A) and Crown Glass(B) of the form $(AB)^5D(AB)^5$ with Air (D) as defect layer with thickness (a) 0.3875 and (b) 0.775 microns (color online)

3. Results and discussions

The photonic band structure of GaP(A) and CG(B) as $(AB)^{10}$ in the near-IR region is considered with normal incidence. Fig. 4 represents the reflectance spectra of GaP-CG PC of structure $(AB)^{10}$ with arrangement as ABABABABABABABABABAB. The reflection curves of PC are plotted with respect to wavelength with the central wavelength being kept equal to 0.6 microns. It can be observed from the figure that the structure displays 100 % reflectivity (zero transmission) where the photonic states are completely not allowed. This complete reflectance arises due to high refractive index of GaP [28]. In addition, the reflectivity band is limited between 0.42 microns to 1 micron. This range of reflectivity is attributed to bandgap of GaP [28].

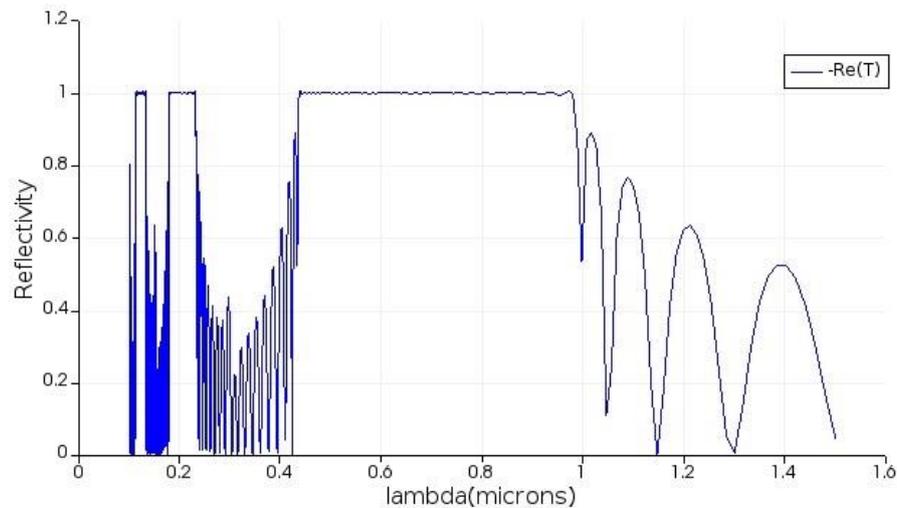


Fig. 4. Reflectance spectra (TE mode) of Photonic crystal of Gallium Phosphide(A) and Crown Glass(B) structure with $(AB)^{10}$ $a=0.042$ microns and $b=0.15$ microns (color online)

In order to observe the effects of defect layer, the PC of Gallium Phosphide(A) and Crown Glass(B) with defect layer with arrangement of $(AB)^5D(AB)^5$ are considered for ZnS and Air one by one. Depending on quarter wave stack condition in PC, the thickness of each defect layer is taken as dissimilar [34]. The thickness here in this case is not taken in continuation with the periodicity of the crystal structure i.e. d_D is not equal to 0.192 microns. In case of ZnS (refractive index=2.3) as the defect material, the width of the defect layer being is taken as 0.1685 and 0.337 microns. Fig. 5 represents the reflectance spectra of $(AB)^5D(AB)^5$ PC with arrangement as ABABABABABDABABABABAB. As a result of the visualization of the curves, it can be seen that there is one defect mode or peak in the 100% reflection region at 1550 nm corresponding to 0.1685 microns defect layer of ZnS. The origin of defect peak in the near-IR region corresponds to presence of defect layer. The presence of defect mode creates an additional energy band layer rendering indirect semiconductor nature of GaP to direct one. When the thickness of ZnS as defect material is doubled, it can be seen in Fig.5 that there are two defect modes at 1279.66 nm and the other at 1967.54 nm. The peak values of defect modes of ZnS as defect layer are tabulated in Table 1.

In case of defect material as Air (refractive index=1), the thickness is again limited by the quarter wave stack condition and, the width of the defect layer was taken as

0.3875 and 0.775 microns respectively. Fig. 6 represents the reflectance spectra of $(AB)^5D(AB)^5$ PC of Gallium Phosphide(A) and Crown Glass(B) with arrangement ABABABABABDABABABABAB. It can be observed from the reflectance spectra of Fig. 6 that there is one defect modes or peak in the 100% reflection region at 1550.28 nm corresponding to 0.1685 microns defect layer of Air due to improved bandgap. Furthermore, when the thickness of Air as defect layer is doubled, it can be seen that there are two defect modes or peaks in the 100% reflection region one at 1297.2 nm and the other at 1925.86 nm. The origin of two peaks for larger thickness of defect layer indicates that defect layer behaves in such a way that the periodicity of the crystal structure doesn't remain intact.

Table 1. Variation of width of various defect material for different thickness with wavelength of defect modes

Defect material	Width of the defect material, d_D (in nm)	Wavelength at which defect mode is obtained (in nm)
ZnS	168.5	1550
	337	1279.66 and 1967.54
Air	387.5	1550.28
	775	1297.2 and 1925.86

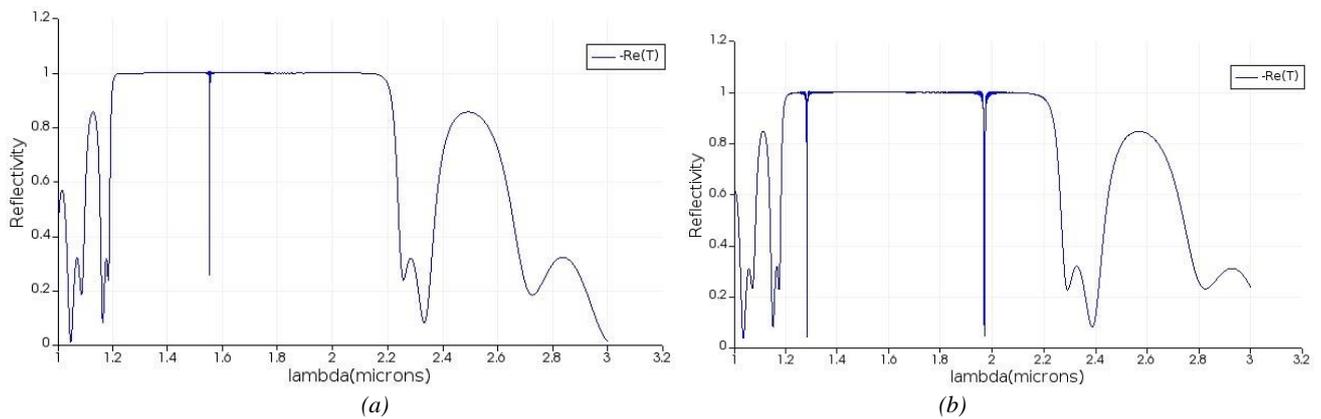


Fig. 5. Reflectance spectra (TE mode) of Photonic crystal of Gallium Phosphide(A) and Crown Glass(B) structure with $(AB)^5D(AB)^5$ with ZnS (D) as defect layer for thickness (a) 0.1685 and (b) 0.337 microns (color online)

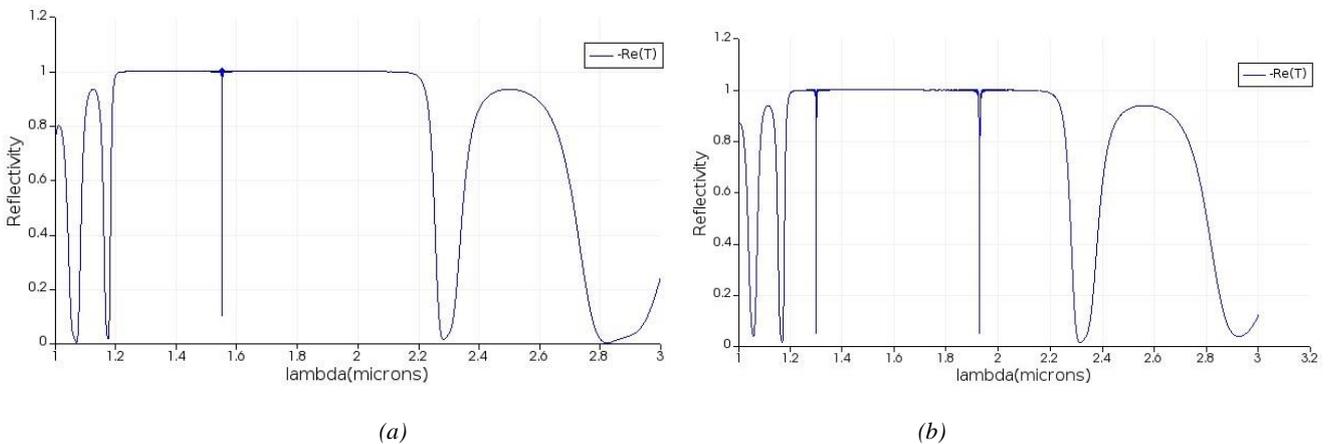


Fig. 6. Reflectance spectra (TE mode) of Photonic crystal of Gallium Phosphide(A) and Crown Glass(B) structure with $(AB)^5D(AB)^5$ with Air (D) as defect layer for thickness (a) 0.3875 and (b) 0.775 microns (color online)

PC structure of GaP and CG with defects are designed in which the defect material and its thickness are varied in order to visualize the defect mode clearly. The defect in our case is introduced not keeping with the periodicity of the crystal structure [23]. Thus, from the visualization of the curves related to defect mode using ZnS and Air as the defect materials, it can be concluded that when the thickness of the defect layer is equal to $d = \text{central wavelength}/4n$, then there exists only one defect mode for both the cases of the defect material [35]. The emergence of single sharp peak in the reflectance spectra of PC of GaP and CG is concordant with propagation of electromagnetic waves in dielectrics [36]. These peaks are referred to as a bound/confined states and makes this PC worthy enough to be employed in optical communications with high frequency carrying capacity [37]. These bound states are capable of fully transmitting the energy in PC matched electromagnetic waves through defect layer via tunneling resonance [38]. However, when the thickness is doubled to $d = \text{central wavelength}/2n$, then there exist two defect modes which can be seen from two peaks in the reflection band region for both the cases of the defect material. The origin of two peaks for larger thickness of defect layer indicates that defect layer behaves in such a way that the periodicity

of PC structure of GaP and CG structure doesn't remain intact. The defect layer of larger thickness is behaving as combination of two defect layers of same ZnS with different thickness. It can be understood that the defect modes of ZnS/Air spreads itself in a way to maximize the concentration of fields in the dielectric defect layer in the PC [39]. These created bound states are the basis for shifting of wavelength to lower and higher magnitude [12]. The same principle is also applicable for higher thickness of air medium as defect layer. The separation between defect modes is slightly more in case of Air as compared to ZnS which could be due to improved resonance in PC. Thus, this PC of GaP and CG can be designed into optical fibers with the light that would be passing through the fiber would be of the near-IR wavelength at which peaks in the 100 % reflection region are obtained. In addition, this PC of Gallium Phosphide and Crown Glass could be also employed in frequency filtering in THz devices as well as optomechanical coupling devices due to induced defect modes.

4. Conclusion

The reflectance spectra of one-dimensional photonic crystal (PC) consisting of alternating layers of Gallium Phosphide and Crown Glass with different defect modes of ZnS and Air were studied with the FDTD simulation. The effect of dielectric layer in PC has been studied for different materials as well as different thickness based on quarter wave stack condition of PC. The PC structure without defect layer exhibited complete reflectance in the near-IR range between 0.42 microns to 1 micron due to high refractive index. The PCs with defect layer exhibited tailored spectra. The PCs with ZnS/Air as defect layer for low thickness exhibit a single resonance defect mode peak due to slight change in periodicity of PC. With doubling the thickness, the reflectance spectra displayed two resonance defect peaks indicating large change in periodicity of PC. The origin of these peaks is in accordance with propagation of electromagnetic waves in dielectric media. These results suggest the importance of PC of Gallium Phosphide and Crown Glass in device applications in photonics, optoelectronics and indicate that this PCs would be revolutionizing the upcoming technology in years to come.

Acknowledgments

This work is not funded by any research agency of India.

References

- [1] S. Hu, S. M. Weiss, *ACS Photonics* **3**(9), 1647 (2016).
- [2] S. M. Weiss, M. Haurylau, P. M. Fauchet, *Optical Materials* **27**(5), 740 (2005).
- [3] Y. Fink, *Science* **282**(5394), 1679 (1998).
- [4] A. Sharkawy, S. Shi, D. W. Prather, *Applied Optics* **41**(34), 7245 (2002).
- [5] A. H. Aly, Z. A. Zaky, A. S. Shalaby, A. M. Ahmed, D. Vigneswaran, *Physica Scripta* **95**(3), 035510 (2020).
- [6] K. A. Amedome Min-Dianey, D. M. Sanogo, N. L. P. Bouana, H. C. Zhang, *Optical Materials* **91**, 1 (2019).
- [7] A. Mouldi, M. Kanzari, *Applied Computational Electromagnetics Society Journal* **26**(3), 259 (2011).
- [8] Z. H. Wu, J. X. Liu, Q. Luo, X. Wen, *J. Optoelectron. Adv. M.* **22**(11), 558 (2020).
- [9] S. Sharma, R. Kumar, K. S. Singh, A. Kumar, *J. Optoelectron. Adv. M.* **19**(5–6), 319 (2017).
- [10] D. Przybylski, S. Patela, *Opto-Electronics Review* **27**(1), 79 (2019).
- [11] H. A. Khan, M. Faryad, *Optik* **180**, 492 (2019).
- [12] M. Sarollahi, S. J. Bauman, J. Mishler, J. B. Herzog, *Journal of Nanophotonics* **10**(4), 046012 (2016).
- [13] Y. Wang, S. Liu, S. Zhong, *Optics Communications* **473**, 125985 (2020).
- [14] S. K. Srivastava, M. Upadhyay, S. K. Awasthi, S. P. Ojha, *Optics and Photonics Journal* **2**(3), 230 (2012).
- [15] V. Mizeikis, S. Juodkakis, R. Tarozaitė, J. Juodkazyte, K. Juodkakis, H. Misawa, *Optics Express* **15**(13), 8454 (2007).
- [16] A. Aghajamali, M. Barati, *Communications in Theoretical Physics* **60**(1), 80 (2013).
- [17] T. C. King, C. J. Wu, *Physica E: Low-Dimensional Systems and Nanostructures* **69**, 39 (2015).
- [18] A. H. Gevorgyan, H. Gharagulyan, S. A. Mkhitarian, *Optik* **180**, 745 (2019).
- [19] V. G. Arkhipkin, V. A. Gunyakov, S. A. Myslivets, V. Y. Zyryanov, V. F. Shabanov, 4th International Conference on Advanced Optoelectronics and Lasers, 183 (2008).
- [20] D. N. Chigrin, A. V. Lavrinenko, D. A. Yarotsky, S. V. Gaponenko, *Journal of Lightwave Technology* **17**(11), 2018 (1999).
- [21] K. Vasudevan, M. C. Divyasree, K. Chandrasekharan, *Optics and Laser Technology* **114**, 35 (2019).
- [22] M. Lin, Z. Ouyang, J. Xu, G. Qiu, *Optics Express* **17**(7), 5861 (2009).
- [23] A. H. Aly, H. A. Elsayed, *Physica B: Condensed Matter* **407**(1), 120 (2012).
- [24] K. Lee, S. H. Song, J. Ahn, *Optics Express* **22**(6), 6269 (2014).
- [25] Ç. Duman, F. Kaburçuk, *Optik* **181**, 993 (2019).
- [26] A. E. Selmy, M. Soliman, N. K. Allam, *Emergent Materials* **1**(3–4), 185 (2018).
- [27] E. Khoobjou, H. Khalesi, V. Ghods, *Optical and Quantum Electronics* **53**(7), 1 (2021).
- [28] K. Schneider, Y. Baumgartner, S. Hönl, P. Welter, H. Hahn, D. J. Wilson, L. Czornomaz, P. Seidler, *Optica* **6**(5), 577 (2019).
- [29] M. Melli, M. West, S. Hickman, S. Dhuey, D. Lin, M. Khorasaninejad, C. Chang, S. Jolly, H. Tae, E. Poliakov, P. St. Hilaire, S. Cabrini, C. Peroz, M. Klug, *Scientific Reports* **10**(1), 1 (2020).
- [30] J. Václavík, D. Vápenka, *EPJ Web of Conferences* **48**, 1 (2013).
- [31] S. Tiwari, S. Jalwania, A. K. Bairwa, *International Journal of Engineering Research and Applications* **2**(4), 186 (2012).
- [32] D. Paul, R. Biswas, N. S. Bhattacharyya, *Indian Journal of Physics* **89**(7), 737 (2015).
- [33] K. Rivoire, Z. Lin, F. Hatami, W. Ted Masselink, J. Vučković, *Optics InfoBase Conference Papers* **17**(25), 22609 (2010).
- [34] M. G. Daher, S. A. Taya, I. Colak, O. M. Ramahi, *Optical and Quantum Electronics* **54**(2), 108 (2022).
- [35] S. K. Srivastava, A. Aghajamali, *Optica Applicata* **49**(1), 37 (2019).
- [36] J. Liu, J. Sun, C. Huang, W. Hu, D. Huang, *Optik* **120**(1), 35 (2009).
- [37] R. Singh, A. Bhargava, *International Journal of Applied Engineering Research* **13**(10), 7616 (2018).
- [38] K. J. Lee, J. W. Wu, K. Kim, *Optical Materials Express* **4**(12), 2542 (2014).
- [39] A. Bhargava, B. Suthar, *Chalcogenide Letters* **6**(10), 529 (2009).

*Corresponding authors: gsharma6@amity.edu;
 sssubramaniam@arsd.du.ac.in;
 shankar3274@gmail.com