Infrared Broadband Reflectors by Nano-Layered Periodic Cryolite/Semiconducting Media

Jyoti Sangwan¹, Deepali Sharma¹, Ram Janma², and Prabal P. Singh², Rajpal Singh³, Narendra Kumar^{1,a}

¹ Department of Physics, SLAS, Mody University of Science and Technology, Lakshmangarh 332311, Sikar, Rajasthan, India.

² Department of Physics, UIET, Chhatrapati Shahu Ji Maharaj University, Kanpur 208024, UP, India.

³ Department of Physics, Govt. M. S. College, Bikaner 334001, Rajasthan, India.

^a nkumar.mu.in@gmail.com

Abstract

This simulation work is based on the analysis of the dispersion characteristics of a nanolayered periodic binary PhC of cryolite and semiconducting layers by using the transfer matrix approach. The dispersion curves and reflection through layered media for optical waves are compared at oblique incidences, and some insights are drawn. It is observed that width of band gap decreases or remains same with increase in the incident angle for 1DPhC, while the bandwidth increases with the normalized frequency at fixed incidence that shows the characteristics of Bragg's gap. The results of the manuscript have promising applications in design of tunable optical filters, broadband reflectors, lasers, and modern communication industry.

Keywords: Nanolayered, Semiconducting, Cryolite, Dispersion, Bragg's gap, Band gap. Received 10 January 2025; First Review 21 January 2025; Accepted 26 January 2025

* Address of correspondence

Dr. Narendra Kumar Department of Physics, SLAS, Mody University of Science and Technology, Lakshmangarh 332311, Sikar, Rajasthan, India.

Email: nkumar.mu.in@gmail.com

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Introduction

Yablonovitch [1] first introduced the photonic band gap for controlling spontaneous emission of light. Before 1987, one-dimensional photonic crystal (1D PhC) in the form of periodic multilayer dielectric stacks were studied extensively and showed that such systems have a one-dimension photonic band gap, spectral range of large reflectivity known as stop band. Leading to these studies, a detailed theoretical study of 1D optical structure was suggested by Vladimir P. Bycov, who was credited the first to investigate the photonic (PBG) on the spontaneous emission from molecule and atom embedded inside the photonic structure.

The periodic modulation of the permittivity occurs in one direction only in such 1D PhCs, where two other directions in the structure are uniform. As an example of such a PhC it can be given is similar to the Bragg grating which that is extensively used in vertical cavity surface emitting lasers as a distributed reflector. These structures are widely used as antireflecting coatings to decrease the reflectance from the surface dramatically and improve the quality of prisms,

lenses, and other optical components. Further Thomas Krauss demonstrated a two-dimensional photonic crystal at optical wavelengths in 1996 [2, 3]. This opened the way to fabricate photonic crystals in semiconductor materials by borrowing methods from the semiconductor industry [3]. The two-dimensional PhCs are commercially used in PhC fiber those were first developed by Philip Russell in 1998, to enhance properties over optical fibers. By 1991, Yablonovitch had demonstrated the first 3DPBG in the microwave regime. The structure was able to produce a drilling array of holes in a transparent material, in which there are holes of each layer form an inverse diamond structure and is known as Yablonovite. Such 3D PhCs have permittivity modulation along all three directions, where the number of possible PhC configurations is much larger than those of 1D or 2D PhCs, and many works were dedicated to the design the new geometric configurations of 3D PhC, which could open new possibilities of their applications [1, 3]. Among them, the most natural 3D PhC is valuable stone opal having its unique optical properties. By turning around, it shows different colours. Although owing to such a peculiar behaviour, ancient people declared that opal had some magic powers, now it is clear that all these

peculiarities are caused by the micro-structure of opal that consists of a number of micro-spheres kept at nodes of facecentred cubic (FCC) lattice.

Although there are three types of PhC and some studies have been made on 2D- and 3D PhCs, the 1DPhC is the simplest one and has been extensively studied by using different types of materials in its binary periodic structure. The properties of metallic PBG materials with introduced defect were reported in microwave frequencies, whose experimental verifications had been made. In brief the PBG materials are composed of air, semiconductors, dielectrics, metals and polymers. By using the transfer matrix method, Kumar and Ojha [5] made an attempt to analyse the reflection properties of a PBG structure with refractive index profile. The reflected broadband in the reflection spectra were compared with the forbidden band-gaps obtained using the analogy of Kronig-Penney model [4, 5] used in the band theory of solids, and some conclusions were drawn. In recent decades, a tremendous amount of work has been devoted to 1DPhC with a variety of materials and structures [6-20]. In this simulation work, we propose a nanolayered periodic PhC of semiconducting media, whose one-layer Sodium hexafluoro aluminate and another is Germanium. We employ the transfer matrix approach for optical waves and reflection through layered media [5, 16].

Theoretical Modelling of Photonic Crystal

Figure 1 shows the binary structure of 1DPhC in which the reflectance of such a structure strongly depends on the radiation incident angle. And the optical properties of such PhC can be determined by the existence of the periodic modulation of the permittivity or the refractive index of the medium. At that, observed effects have strong analogy to the solid state, i.e., the periodically arranged structure of atoms in crystal lattice.

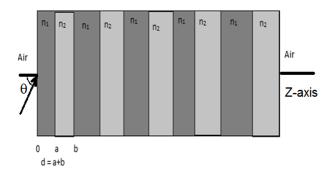


Figure 1: Periodic variation of 1DPhC structure.

We consider the EM wave propagation along x-axis through the structure, the periodic refractive is [4]

$$n(z) = \begin{cases} n_1, b < z < d \\ n_2, 0 < z < b \end{cases}$$
 (1)

with $n_1(z+d) = n_1$ and $n_2(z+d) = n_2$, and d = a+b be the lattice period, with a and b as the widths of the two layers whose refractive indices are n_1 and n_2 , respectively.

The 1D EM wave equation for the spatial part of the eigen mode is expressed as

$$\frac{d^2 E(z)}{dz^2} + \left[\left(\frac{\omega}{c} n \right)^2 - \beta^2 \right] E(z) = 0 \qquad , \quad (2)$$

The electric field distribution E(x) within each layer can be expressed as the sum of an incident and reflected plane waves, and so in the m^{th} unit cell it is written as

$$E(z) = \begin{cases} a_m e^{-ik_1(z-md)} + b_m e^{ik_1(z-md)}; & (md-a) < z < md \\ c_m e^{-ik_2(z-md+a)} + d_m e^{ik_2(z-md+a)}; & (m-1)d < z < (md-a) \end{cases}$$
, (3)

in which a_m , b_m , c_m , and d_m are constants.

We define,

$$k_i = \left[\left(\frac{\omega}{c} n_i \right)^2 - \beta^2 \right]^{1/2} = \frac{n_i \omega}{c} \cos \theta_i; i = 1, 2, \text{ where}$$

 θ_1 and θ_2 are the ray angles in the consecutive layers.

Assuming θ as the angle of incidence,

$$\cos \theta_i = \left(1 - \left(\frac{1}{n_i}\right)^2 \sin^2 \theta\right)^{1/2}$$
. With the help of TMM,

we have the relation [4, 5]

$$\begin{pmatrix} a_{m-1} \\ b_{m-1} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} a_m \\ b_m \end{pmatrix} , \tag{4}$$

where the matrix elements are expressed as

$$\begin{split} A_{11} &= \exp(+ik_1a) \Bigg[\cos k_2b + \frac{1}{2}i \bigg(\frac{k_2}{k_1} + \frac{k_1}{k_2} \bigg) \sin k_2b \Bigg], \\ A_{12} &= \exp(-ik_1a) \Bigg[\frac{1}{2}i \bigg(\frac{k_2}{k_1} - \frac{k_1}{k_2} \bigg) \sin k_2b \Bigg], \\ A_{21} &= \exp(+ik_1a) \Bigg[-\frac{1}{2}i \bigg(\frac{k_2}{k_1} - \frac{k_1}{k_2} \bigg) \sin k_2b \Bigg], \text{ and } \\ A_{22} &= \exp(-ik_1a) \Bigg[\cos k_2b - \frac{1}{2}i \bigg(\frac{k_2}{k_1} + \frac{k_1}{k_2} \bigg) \sin k_2b \Bigg]. \end{split}$$

Since equation (4) above is unimodular

 $A_{11}A_{22} - A_{21}A_{12} = 1$. By using Floquet theorem [4-6]

$$K(\beta, \omega) = \frac{1}{d}\cos^{-1}\left[\frac{1}{2}(A_{11} + A_{22})\right]$$
 (5)

Thus, the dispersion relation (ω versus K) will be

$$cos(Kd) = cos(k_1a)cos(k_2b) - \frac{1}{2} \left[\frac{k_2}{k_1} + \frac{k_1}{k_2} \right] sin(k_1a) sin(k_2b)$$
(6a)

Hence,

$$cos(Kd) = cos(k_1a) cos(k_2b) - \frac{1}{2} \left[\frac{n_2}{n_1} + \frac{n_1}{n_2} \right] sin(k_1a) sin(k_2b)$$
(6b)

Reflectance (R_N) of the 1DPhC can be obtained by [4, 16]

$$R_{N} = \frac{|A_{21}|^{2}}{|A_{21}|^{2} + \left(\frac{\sin Kd}{\sin NKd}\right)^{2}},\tag{7}$$

where A_{2I} is matrix element and N is total number of unit cells. For a lossless media, the transmission can be obtained as $T_N = 1 - R_N$.

Results and Discussion

For the numerical calculations in our study, we have taken Na₃AlF₆ and Ge as n_1 =1.34 and n_2 =4.2 [11, 16], and their thicknesses are d1=360nm and d2=120nm, respectively [11], where d is the total stack thickness. The dispersion relation for a structure have been derived with Bloch equation as by the equation (6b) and the reflection and transmission can be obtained by the equation (7), respectively. We now plot dispersion curves and reflection spectra at incident angles 0° , 20° and 60° .

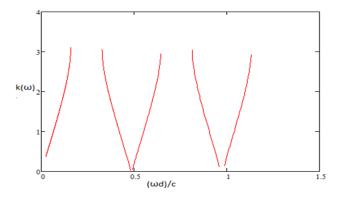


Figure 2: Plot of the dispersion relation as a function of normalized frequency for the 1DPhC at incident angle $\theta = 0^{\circ}$

Figures 2, 3, and 4 represent the dispersion relation curves i.e. $k(\omega)$ versus normalized frequency, $\omega d/c$ i.e., of the structure for different oblique angle of incidences $\theta = 0^{\circ}$,

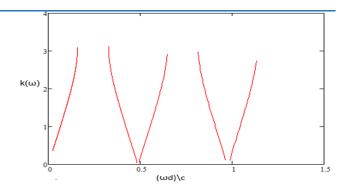


Figure 3: Plot of the dispersion relation as a function of normalized frequency for the *1DPhC* at incidentangle $\theta = 20^{0}$ [16].

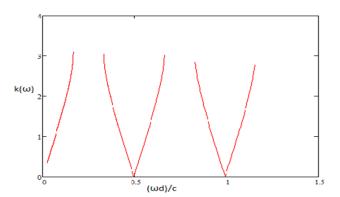


Figure 4: Plot of the dispersion relation as a function of normalized frequency for the IDPhC at incidentangle $\theta = 60^{0}$

 20° , 60° . It is clear that the bandwidths of odd numbered forbidden band gaps are wide but the bandwidths of even numbered forbidden band gap are extremely narrow. It is noticeable here that the lattice constant d is arbitrary; thus, the result obtained here is only valid for arbitrary wavelengths and the existence of band gap is possible d is nearer to λ , i.e., when the normalized frequency is perpendicular.

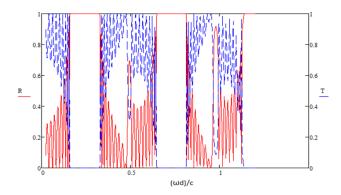


Figure 5: Plot of Reflection and Transmission as a function of normalized frequency for the *IDPhC* attncident angle $\theta = 0^0$.

From Figures 5, 6, and 7, it is noted that the first and third band gap shows the hundred percent reflection therefore the transmittance is zero. i.e. at these frequencies, the waves are completely reflected and do not pass through the crystal but

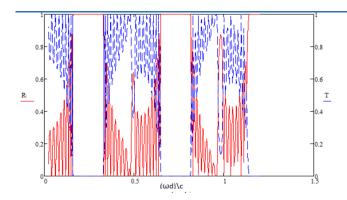


Figure 6: Plot of Reflection and Transmission as a function of normalized frequency for the *IDPhC* attncident angle $\theta = 20^{\circ}$.

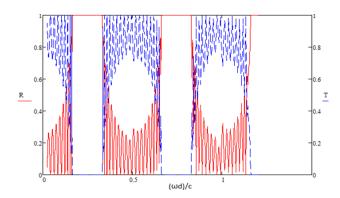


Figure 7: Plot of Reflection and Transmission as a function of normalized frequency the IDPhC attncident angle $\theta = 60^{\circ}$.

in second and fourth band gaps, the transmittance is not zero, which means part of the wave can pass.

Table 1: Normalized Frequency Range at Incident Angle 0° .

S. No. of Bands	Band Gap (Dispersion Curves)	Complete Reflection Range	Bandwidth
1	1.2-1.37	1.2-1.37	0.17
2	0.808-0.65	0.808-0.65	0.158
3	0.327-0.164	0.324-0.164	0.163

Table 2: Normalized Frequency Range at Incident Angle 20° .

S. No. of Bands	Band Gap (Dispersion Curves)	Complete Reflection Range	Bandwidth
1	1.2-1.143	1.2-1.143	0.057
2	0.811-0.652	0.811-0.652	0.159
3	0.324-0.163	0.324-0.163	0.161

From the bandwidth listed in Tables at three incident angles, it is observed that the bandgap obtained from the dispersion curves and reflection spectra are analogous and mostly same. As the incident angle increases, the width of band

gap, in terms of the normalized frequency ranges for 1DPhC, decreases or remains same. However, at fixed incidence, the bandwidth increases with the normalized frequency.

Table 3: Normalized Frequency Range at Incident Angle 60° .

S. No. of Bands	Band Gap (Dispersion Curves)	Complete Reflection Range	Bandwidth
1	1.2-1.165	1.2-1.165	0.035
2	0.822-0.667	0.822-0.667	0.155
3	0.327-0.164	0.327-0.164	0.163

Conclusion

The present work is dedicated to an analysis of a nanolayered structure, considering as a simple model of 1D semiconducting photonic crystal. From the dispersion curves, it is found that the structure with chosen refractive index profiles and lattice parameters exhibits allowed and forbidden bands. It is mentioned that with increase in the incident angle, the bandwidth for 1DPhC either decreases or remains same. However, at fixed incidence, the bandwidth increases with the normalized frequency. This study can be useful in design of tunable optical filters, nano-optics and may have promising applications in modern communication industry, lasers and optical computing.

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