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Abstract
In this contribution, a binary photonic crystal, basically comprising repeated layers of quartz and silicon, is studied analytically using transfer matrix method. Refractive indices of the constituent layers are assumed to depend on wavelength according to Sellmeier approximation formula. The effect of the selected materials, number of layers and their thicknesses and the angle of incidence on transmittance of the photonic crystal are studied in detail. Results show that the structure is more sensitive to changes in silicon layer thickness and tolerant to changes in the incident angles. Changing the layer thickness, multi photonic band gaps arise and the gaps are shifted to another optical frequency range. As the difference between refractive indices gets larger, the photonic band gap (PBG) gets wider and moves toward longer wavelengths. These photonic crystals are expected to be useful in fabricating perfect mirrors, designing optical control devices and optical sensors.

1. Introduction

A Photonic crystal (PC) is an artificial structure of alternative periodic refractive indices exhibiting forbidden regions analogous to the electronic band nature in solids and quantum wires [1–3]. Soon after the first photonic crystals (PCs) have been introduced by Yablonovitch and John in the 1980’s [4, 5], they have grabbed an increasing attention due to their ability to control propagation of electromagnetic waves within the layers [6–8]. It was found that the modulated refractive index structures show peculiar propagation features similar to refraction in geometrical optics using some unusual media [1, 2, 9–13]. The PC structure is usually fabricated in such a way that the propagation direction of light waves can be steered or even forbidden upon changing wavelength, layers thicknesses or the angle of incidence [13]. The spectral range in which electromagnetic waves cease to propagate is called the photonic band gap (PBG). Existence of such (PBGs) is understood as being arising from multiple Bragg scattering within the layers [3–5, 14–16]. Together with the property of having multi PBGs, most PC types are important in solid state and optical physics applications such as perfect reflectors, flip flops, optical logic switches, optical filters, laser’s optical cavity mirrors, optical and pressure sensors [17–26], him. As optical polarizers, PCs have been reported to be suitable in high power laser arrangements. Such polarizers are preferred over the conventional ones because the absorption is negligible and the device can operate not only at Brewster’s angles but also in a much wider angular range [2].

Because of their significant sensitivity and neatness, a great effort has been oriented to establishing optical sensors based on PCs especially those comprising defects [27]. The sensing process in PCs depends mainly on the changes in output power and the shift of PBGs due to changes in refractive indices [28, 29].

In general, PBG width is considerably affected by the number of periods, individual thicknesses of layers and their refractive indices [30–33]. In addition, the constituent materials of a PC can affect its performance. Dielectrics, metals, nanocomposite materials, plasmas, superconductors and left handed materials are usually used [2, 32–36].

Most of the reported studies assume different classes of materials with only averaged refractive indices in the spectral range of interest. In our discussion, however, we adopt 1D binary planar PCs comprising media with
spectral dependent refractive indices so as to be more realistic. Adopting 1D binary planar photonic crystals gives simplicity and ease of manufacturing over 2D, 3D or annular PCs. The refractive indices dependence are assumed to follow Sellmeier approximation [37]. Our contribution is designated as follows: A theoretical formulation of the problem is given in section 2. Basically, the transfer method approach is discussed in this section. In section 3, numerical results and discussion are carried out. This section is devoted to explore the effect of some parameters on the output of our structure. Conclusion remarks and findings are given in section 4.

2. Theoretical formulation

As schemed in figure 1 below, TE plane electromagnetic waves, with electric field directed along y-axis, are incident to the face of the uppermost dielectric slab of a binary photonic crystal consisting of N periods. Each period comprises two layers of widths $h_1$ and $h_2$ and refractive indices $n_1$ and $n_2$; respectively. All media are supposed to be nonmagnetic so that relative permeability is unity.

At each interface, part of the wave reflects and the other part emerges to the next slab and so on. The transverse electric field (with $e^{i(kz-\omega t)}$ dependence) within the $j^{th}$ layer is given as:

$$E_j = A_j e^{ik_j x} + B_j e^{-ik_j x}$$

(1)

where, $k_j = \sqrt{k_1^2 n_1^2 - \beta^2} = k_1 n_1 \sin \theta_j$; $j = 0, 1, 2$ and $\beta = k_2 n_2 \cos \theta_j$ is the propagation constant along the z-axis and $\theta_j$ is the angle of incidence. The amplitudes $A_j$’s and $B_j$’s can be calculated through the boundary conditions.

The z-component of the magnetic field can be calculated from the relation [38]: $H_z = -\frac{i}{\omega} \frac{\partial E_j}{\partial z}$ so that one writes:

![Figure 1. Schematic of the proposed 1D binary photonic crystal.](image-url)
\[
H_j = \frac{k_j}{\omega \mu_j} (A_j e^{ik_j x} - B_j e^{-ik_j x})
\]  

Here, \(\mu_j = \mu_i\) for all layers.

The transmission matrix \(T_{12}\) relating the fields at both sides of the interface between the first interface between layer 1 and layer 2 is well known in literature [2, 39, 40]. It is given as:

\[
T_{12} = \frac{k_1 + k_2}{2k_1} \begin{pmatrix}
1 & \frac{k_1 - k_2}{k_1 + k_2} \\
\frac{k_1 - k_2}{k_1 + k_2} & 1
\end{pmatrix} = \frac{1}{t_{12}} \begin{pmatrix}
1 & \tau_{12} \\
\tau_{12} & 1
\end{pmatrix}
\]  

Such that: \(\tau_{12}, \tau_{12}\) are the Fresnel transmission and reflection coefficients. Electromagnetic fields transmitting to the second layer and propagating within are related through the propagation matrix \(P_2\) [39, 40]:

\[
P_2 = \begin{pmatrix}
e^{ik_2h_2} & 0 \\
0 & e^{-ik_2h_2}
\end{pmatrix}
\]  

Consequently, the transfer matrix \(M_{12}\) is attained:

\[
M_{12} = T_{12}P_2 = \frac{1}{t_{12}} \begin{pmatrix}
1 & \tau_{12} \\
\tau_{12} & 1
\end{pmatrix}\begin{pmatrix}
e^{ik_2h_2} & 0 \\
0 & e^{-ik_2h_2}
\end{pmatrix} = \frac{1}{t_{12}} \begin{pmatrix}
e^{ik_2h_2}e^{-ik_1h_1} & \tau_{12}e^{-ik_1h_1} \\
\tau_{12}e^{ik_1h_1} & e^{ik_2h_2}
\end{pmatrix}
\]  

Again, the electromagnetic waves arriving at the next interface will be matched and we end with another transmission matrix \(T_{21}\) and another propagation matrix \(P_1\). The resultant transfer matrix \(M_{21}\) then reads:

\[
M_{21} = T_{21}P_1 = \frac{1}{t_{21}} \begin{pmatrix}
e^{ik_1h_1} & \tau_{21} \\
\tau_{21} & 1
\end{pmatrix}\begin{pmatrix}
e^{ik_1h_1} & 0 \\
0 & e^{-ik_1h_1}
\end{pmatrix}
\]  

Notice that \(\tau_{21} = -\tau_{12}\).

The resulting transfer matrix for the first period of our crystal is then:

\[
M = T_{12}P_2T_{12}P_1 = M_{12}M_{21} = \frac{1}{t_{12}t_{21}} \begin{pmatrix}
e^{ik_2h_2} & \tau_{12}e^{-ik_1h_1} \\
\tau_{12}e^{ik_1h_1} & e^{ik_2h_2}
\end{pmatrix}\begin{pmatrix}
e^{ik_1h_1} & \tau_{21} \\
\tau_{21} & 1
\end{pmatrix}\begin{pmatrix}
e^{ik_1h_1} & 0 \\
0 & e^{-ik_1h_1}
\end{pmatrix}
\]

Multiplying the matrices and rearranging, matrix elements can be expressed as:

\[
M_{11} = \frac{1}{t_{12}t_{21}} \left( e^{i(\phi_1 + \phi_2)} - \tau_{12}^2 e^{i(\phi_1 - \phi_2)} \right) \quad M_{12} = \frac{\tau_{12}}{t_{12}t_{21}} \left( e^{-i(\phi_1 + \phi_2)} - e^{-i(\phi_1 - \phi_2)} \right)
\]

\[
M_{21} = \frac{\tau_{21}}{t_{12}t_{21}} \left( e^{i(\phi_1 + \phi_2)} - e^{i(\phi_1 - \phi_2)} \right) \quad M_{22} = \frac{1}{t_{12}t_{21}} \left( e^{-i(\phi_1 + \phi_2)} - \tau_{21}^2 e^{-i(\phi_1 - \phi_2)} \right)
\]

Where, \(\phi_1 = k_1h_1, \phi_2 = k_2h_2\).

With the last layer chosen to be the same as layer 1, the transfer matrix of the stacks will be:

\[
m = T_{12}P_2T_{12}P_1T_{12}P_1T_{12}P_1 \ldots T_{12}P_2T_{12}P_1 = M_{12}M_{21}M_{22}M_{12} \ldots M_{12}M_{21} = M^N
\]

Since \(M\) is unimodular (\(|M| = 1\)), the power matrix \(M^N\) can be written from Chebyshev polynomials [2, 40, 41] as:

\[
m = (M)^N = \begin{pmatrix} M_{11}U_{N-1}(X) - U_{N-2}(X) & M_{12}U_{N-1}(X) \\ M_{21}U_{N-1}(X) & M_{22}U_{N-1}(X) - U_{N-2}(X) \end{pmatrix}
\]

\(U_N\) denotes Chebyshev polynomials of the second kind and they are given by:

\[
U_N(X) = \frac{\sin((N + 1)\cos^{-1}X)}{\sqrt{1 - X^2}} ; \quad X = \frac{1}{2}(M_{11} + M_{22})
\]

The incident, reflected and transmitted fields can then be written as:

\[
\begin{pmatrix} E_0 \\ rE_0 \end{pmatrix} = M_{01}(M)^N T_{22N+1}(X) \begin{pmatrix} tE_0 \\ 0 \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} tE_0 \\ 0 \end{pmatrix}
\]

with:

\[
M_{01} = T_{01}P_1 = \frac{1}{t_{01}} \begin{pmatrix} 1 & \tau_{01} \\ \tau_{01} & 1 \end{pmatrix}\begin{pmatrix} e^{ik_1h_1} & 0 \\
0 & e^{-ik_1h_1}
\end{pmatrix} = \frac{1}{t_{01}} \begin{pmatrix} e^{ik_1h_1} & \tau_{01}e^{-ik_1h_1} \\
\tau_{01}e^{ik_1h_1} & e^{-ik_1h_1}
\end{pmatrix}
\]
and,

$$T_{2N+1} = \frac{1}{t_0} \left( \frac{1}{t_0} - \frac{1}{r_0} \right)$$

(14)

Using $T$ instead of $M$ in the last medium is justified since we are interested only in the fields just transmitting out of the structure.

Having evaluated $a$, $b$, $c$ and $d$, the Fresnel's coefficients can be obtained and both reflectance and transmittance can be evaluated $[2, 41, 42]$:

$$T = t^n = \left| \frac{1}{a} \right|^2 = \frac{t_0 h_0}{(m_1 - r_0 m_1) e^{ik h_1} + (m_2 - r_0 m_2) e^{-ik h_1}}$$

(15)

$$R = r^n = \left| \frac{c}{a} \right|^2 = \frac{(m_1 - r_0 m_2) e^{ik h_1} + (m_2 - r_0 m_2) e^{-ik h_1}}{(m_1 - r_0 m_1) e^{ik h_1} + (m_2 - r_0 m_2) e^{-ik h_1}}$$

(16)

3. Results and discussion

Each period of our 15-period PC consists of two layers the first of which is quartz ($\alpha - \text{SiO}_2$) whereas the second layer is silicon. At optical frequencies, however, semiconductors follow dielectric behavior because the electron hole excitation is ineffective $[43]$. In figure 2, the effect of choosing the refractive index (simply the constituent materials) on the transmittance spectrum is shown. Four materials, namely; YAG ($\text{Yttrium aluminum garnet}$, $\text{Y}_3\text{Al}_5\text{O}_{12}$), $\text{ZrO}_2:12\%\ Y_2\text{O}_3$, $\alpha - \text{ZnS}$, and silicon are used as the second layer in our PC. The permittivity of all materials are computed at about 25 °C through Sellmeier approximation formula:

$$\varepsilon = A + \frac{B \lambda^2}{\lambda^2 - C} + \frac{D \lambda^2}{\lambda^2 - E}$$

(17)

where, $\lambda$ is the wavelength in $\mu$m. Sellmeier coefficients $A$, $B$, $C$, $D$ and $E$ (valid specifically for the optical range of wavelengths) of the proposed materials are given in table 1.

As the refractive index of the second layer increases, the photonic band gap PBG gets wider and is shifted to the right towards the region of higher wavelength. When silicon is used, all visible light ceases to propagate within the crystal. This is why we’ll adopt silicon in all coming analysis. On the other hand PC comprises YAG layer is promising for solar cells coating since the transmission is almost unity over the visible range.
The dashed plots in figure 2 represent the transmittance of the proposed PC with constant non-dispersive materials. In all four substances used as second layer of our PC, it is only silicon that affects transmittance apparently. In fact, the dispersive material exhibits a narrower \( \text{PBG} \). Forbidden bands emerge a bit to the UV region in case of only adopting the averaged refractive indices.

In figure 3(a) we carry out a comparison between transmittance of a 9-period PC for different constituents. The first layer is always quartz. It is apparent that as refractive index increases, the minimum transmittance is more quickly attained. In the case of \( \text{YAG} \) and \( \text{ZrO}_2:12\% \text{Y}_2\text{O}_3 \), \( \text{PBGs} \) do not even appear. \( \text{PBG} \) in case of \( \alpha\)-\( \text{ZnS} \) is hardly constructed but it is well established in case of silicon as a second layer.

In figure 3(b), transmittance for the four used materials with quartz as first layer is shown. As simply predicted from figures 2 and 3(a), the first material (\( \text{YAG} \)) is always much farther than constructing a \( \text{PBG} \). Transmittance of this structure reaches \( 95\% \) in average. Although fluctuating, this structure is potentially promising for solar cells coating with minimal number of PC layers. The second material (\( \text{ZrO}_2:12\% \text{Y}_2\text{O}_3 \)) is very close to have a band gap but it cannot reach a stopping condition. Transmittance reaches roughly 0.05 and then begins to increase again. In both \( \alpha\)-\( \text{ZnS} \) and silicon, it is possible to have \( \text{PBGs} \). About 12 periods are required in case of \( \alpha\)-\( \text{ZnS} \) while nearly 8 are required in case of silicon. The quartz-silicon structure prohibits all visible radiation so that it is very efficient in designing perfect reflecting mirrors.

To see how thickness of the layers affects the structure output, the transmittance is plotted against several thicknesses of quartz and silicon layers as shown in figures 4(a) and (b). It is clear that the \( \text{PBG} \) is rapidly shifted to the right due to relatively small changes in the silicon layer. Changing the silicon thickness of just 20 nm (from 30 nm to 50 nm) results in about 480 nm shift to the right, this shift could be calibrated to be used in temperature or pressure sensors. On the other side, when quartz thickness is changed by 100 nm (from 80 nm to 180 nm), the \( \text{PBG} \) is only shifted by 350 nm. This means that the structure is more sensitive to changes in the silicon layer thickness. Accordingly, changing \( h_2 \) can play an effective role in designing tunable controllable optical sensing devices. Another very promising property arising here is that changing thickness gives rise to

![Figure 3](image-url)
appearance of multi-band gaps. Specifically, two gaps appear at \( h_1 = 100 \) nm in figure 4(a) whereas 3 photonic gaps arise in figure 4(b) at \( h_2 = 50 \) nm. This is very important in establishing some devices such as flip flops and optical switches.

It is beneficial at this point to check how the boundaries of \( PBG \) responds to changes in layer thicknesses. Dependence on thickness is found to be very close to a linear behavior as shown in figure 5. In figure 5(a), the lower and upper lines have slopes 2.38 and 3.35 respectively whereas in figure 5(b) the slopes are 5.87 and 8.70. Additionally, the change of \( PBG \) width with respect to change in thickness is calculated to be 0.97 in case of quartz and it is 2.83 in case of silicon. This assures that the structure is much more sensitive to changes in silicon layer thickness. This is supposed to be helpful in fabricating controllable optical sensors.

The proposed \( PC \) structure under consideration is tolerant to changes in the angle of incidence. It is clear from figure 6 that only 50 nm shift to the right occurs when the angle of incidence changes from zero (normal incidence) to \( 60^\circ \). At the same time, it is just a few nanometers shift to the left. That is, one may have nearly the same output no matter how the crystal is exposed to light. This is supposed to be very effective in implementing perfect mirrors.

Figure 4. (a) Transmittance against wavelength of quartz-silicon binary PC at different quartz thicknesses the silicon thickness is fixed to 35 nm. (b) Transmittance against wavelength of the structure at different silicon thicknesses. The quartz thickness is fixed to 80 nm. \( N = 15 \).

Figure 5. Dependence of \( PBG \) boundaries on layer thicknesses: (a) against quartz layer changes and (b) against silicon layer changes.
4. Conclusion

Using the transfer matrix, the proposed PC is studied theoretically and the subsequent numerical results within the optical wavelengths are discussed. The width of the PBG is shown to depend on the materials used and their thicknesses. PCs comprising silicon as the second layer in the period exhibit optimum properties. This is related to the highest difference between the constituent refractive indices. These PCs are very sensitive to silicon thickness compared with Quartz, the first layer in the period. Upon changing thickness, the PBGs are shifted to other frequency (wavelength) regions. The width of the gap is also affected. At some thickness, more than one gap appears in the region of study. The structure shows low sensitivity to the angle of incidence with a slight shift towards the lower wavelength region. Silica-YAG structure exhibits a significantly high transmittance in the visible region so that it is a real good candidate for solar cells coatings. Such PCs may be beneficial in constructing controllable optical devices. Moreover, they can be used to control the propagation of electromagnetic radiation and fabricating perfect mirrors and reflectors [44].

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Figure 6. Transmittance against wavelength for quartz-silicon binary PC at different angles of incidence. h1 = 80 nm, h2 = 35 nm and N = 15.
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