Refractive index EV sensor based on conventional and mirror image 1D defective photonic crystal designs: theoretical study

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Abstract
In the present study, we have theoretically investigated the sensing and detection mechanism of refractive index of various samples containing extracellular vesicles by using the conventional and mirror image 1D defective photonic crystal designs. The transfer matrix method has been used to analyze the transmission properties of both structures at normal incidence. The performance of the proposed designs has been examined by measuring the shift in the position of the defect mode inside PBGs of respective structures depending upon the corresponding change in refractive index of various EV samples. The comparison between the observed data with the experimentally available standard data may be used to find out refractive index of unknown EV samples. Moreover, mirror image 1D defective PC design can be used as an alternative of one-dimensional annular photonic crystal without defect with air core in which propagation of electromagnetic waves is only along the radial direction. Finally, we have compared the sensing and detection features of both the designs made up of a conventional and mirror image 1D defective PCs. It has been noticed that the mirror image defective structure provides a narrow transmission peak of unit transmittance inside the PBG. This remarkable feature of mirror image one-dimensional defective photonic crystal design may be utilized to develop various highly sensitive sensors. The figure of merit and quality factor values of the proposed design are high and low, respectively. Such high performance bio-sensor with better sensing capabilities may be very useful in chemical and biological sample detection.

Keywords Photonic crystal · Transfer matrix method · FOM · Sensor

1 Introduction
MATLAB based computational techniques can be applied to simulate the performance of the photonic devices composed of one dimensional (1D) photonic crystals (PCs) [1] with the help of transfer matrix method (TMM). Basically 1D PCs are multilayer layer periodic structures which can tremendously control the propagation of incident light passing through the structure and have intriguing optical properties. Such intriguing properties of the photonic structure are dependent upon the refractive index of the constituent material layers of the structure. The Bragg scattering of light through the interfaces of photonic structures results the formation of forbidden energy gap which is called as photonic bang gap (PBG) [2, 3]. The incident electromagnetic radiation with frequency lies inside PBG does not allow to pass through the structure and allows rest of the frequencies to pass through the structure. This property of controlling the propagation of light passing through the photonic structure has found interesting for the development of 1D PC assisted next generation photonic devices capable of doing multi-tasking. The correlation between PBG and photon was first established by two pioneer scientists Yablonovitch and John in 1987 [4, 5]. Undoubtedly nowadays the field of photonic research has become new hotspot due to high accuracy, cost effective and robust nature of photonic devices which have useful applications in thermal, optical, biological and
biomedical engineering and technologies [6–9]. The disturbance in periodicity of photonic structure may lead to the existence of tunneling mode of high transmittance also called as defect mode inside PBG of the photonic structure [10–12]. This property of defect mode is very useful for designing of photonic sensing devices equipped with special features whose position and intensity is dependent upon the refractive index of defect layer region [13, 14]. Additionally diversified applications of 1D defective PCs have strengthened their role of designing of photonic biosensors in contrast to conventional PCs without defect. Moreover, the ease of fabrication involved with 1D PCs in addition to rapid and instant detection capabilities along with the real establishment make them suitable as compared to two-dimensional (2D) and three-dimensional (3D) PCs [15, 16]. The photonic biosensing devices work on the minute refractive index change detection principle of sample to be poured into cavity region of the device. Some of the important biosensing applications of photonic sensors are food sensor, sugar concentration sensor, milk density sensor, nutrition sensor, etc. Beside this in biological photonic sensing scheme, molecule assisted refractive index is considered which can be extended as liquid sensor, hemoglobin sensor, glucose sensor but it is not limited for food and agriculture industry only [17, 18]. Photonic biosensors provide early stage diagnosis of diseases by investigating samples consisting of urine albumin, glucose identification, biomarker, creatinine and cancer cell [19–22]. Moreover, photonic sensing requires less volume of sample under investigation in comparison to conventional sensing technology [19, 20, 23, 24].

Motivated by aforementioned piece of excellent research work [12–23] in this paper we are proposing a sensor for detection of refractive index of various samples containing extracellular vesicles (EVs) by using conventional and mirror image 1D defective photonic crystal designs. Though the conventional optical technologies are utilized to measure size and count of extracellular vesicles with the help of their refractive indices, it is difficult to measure refractive indices of EVs because conventional methods require accurate knowledge of size of EVs and light scattering. Moreover, most of the EVs have their diameter which is smaller than the wavelength of visible light to be used in light microscopy. Thus, light microscopy process could not able to resolve EVs [24]. The proposed designs are capable of measuring the shift in position of the defect mode inside PBGs which depending upon change of refractive index for various EV samples and also by comparing the observed data with the experimentally available standard data of EVs with the help of their refractive index values [24, 25]. To the best of our knowledge, the 1D defective PC based refractive index EV sensor has been used for the first time to detect the cell count in order to assess the nutrient balance human body. The organization of the proposed work is as follows: Sect. 2 introduces the theoretical formulation behind the problem based on transfer matrix method (TMM) [26–34]. Section 3 presents the numerical results and discussions pertaining to the work, at last calculations are presented in Sect. 4.

2 Theoretical formulation of proposed refractive index sensor design

The proposed 1D periodic, defective photonic structures consisting of single and double defect layers are shown in Fig. 1a, b and c, respectively. The electromagnetic waves, making an incident angle \( \theta_0 \) with respect to the z-axis, are assumed to be normal. The above designs are assumed to have alternating layers A and B of refractive index \( n_A \) and \( n_B \) of thickness \( d_A \) and \( d_B \), respectively. The defect layers \( C \) of thickness \( d_C \) and \( 2d_C \) of refractive index \( n_C \) has been created in the middle of 1D periodic structure \((AB)^N\) to form two different 1D defective PC structures \((AB)^N C(AB)^N\) and \((AB)^N C C(BA)^N\), respectively (Table 1). These defect layer regions are filled with various EV samples of different refractive index under investigation as per the data given in Table 2. The theoretical investigations based on TMM have been carried out to study the propagation of light through the proposed 1D defective PC structures as \((AB)^N C(AB)^N\) and \((AB)^N C C(BA)^N\) in visible region at normal incidence [26–34]. Here, \( N \) is representing the total number of periods. The interaction between the incident electromagnetic radiation and the proposed structure is described by means of transfer total matrix as under

\[
M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = \begin{pmatrix} m_A m_B \end{pmatrix}^{N/2} m_C \begin{pmatrix} m_A m_B \end{pmatrix}^{N/2} \tag{1}
\]

where \( M_{11}, M_{12}, M_{21}, \) and \( M_{22} \) are representing the elements of total transfer matrix of whole structure inclusive of respective defect layers. The characteristic matrix of layers \( A, B \) and \( C \) of materials silicon, polystyrene and samples containing EVs, respectively, are described below.
The value of \( p \) associated with layers A, B and C are at
\[ p_A = n_A, \quad p_B = n_B \quad \text{and} \quad p_C = n_C. \] 

The transmission coefficient based on Chebyshev polynomial of second kind is calculated as [26–34]
\[ t = \frac{2p_0}{(M_{11} + M_{12}p_f)p_f + (M_{21} + M_{22}p_f)} \] 

Here \( p_0 = p_f = n_0 \), since the entire structure is surrounded by air of refractive index \( n_0 \). Finally, the transmittance of the proposed designs can be obtained with the help of following relation as [26–34]
\[ T = \left. \left| \frac{p_f}{p_0} \right| \right|^2. \] 

The proposed biosensing designs are composed of 1D defective PCs (AB)^3C(AB)^4 and (AB)^3C(AB)^4 of single and double defect layers, respectively. We have named the second design (AB)^3C(AB)^4 as a ring mirror structure [25] which is consisted of 1D defective planar PC of optical characteristics which are identical to the optical characteristics of 1D APCs without defect when the propagation of electromagnetic waves is along the radial direction. In this section first we elaborate design of the 1D planar photonic crystal structure (AB)^N composed of alternating layers A and B of materials silicon and polystyrene, respectively, as shown in Fig. 1a. Here, \( N \) represents total number of periods of the structure (AB)^N. For sensing and detecting of different EV samples, we modify the above photonic structure (AB)^N by creating a single and double cavity regions C and CC in the middle of structure to create two different 1D defective photonic crystals (AB)^N2C(AB)^N2 and (AB)^N2CC(AB)^N2 respectively. The pictorial representation of single and double defect photonic structures (AB)^N2C(AB)^N2 and (AB)^N2CC(AB)^N2 is shown in Fig. 1b and c, respectively. The ambient medium around both the structure is air. The various biomedical and chemical fluids under investigation have to be poured through the opening embedded into the upper surface of both the structures as shown in Fig. 1b and c. The proposed research work has been carried out in visible region of electromagnetic spectrum under normal incidence \( (\theta_0 = 0^\circ) \) to overcome the difficulties associated with oblique incidence. The numeric values of different structural parameters associated with both the structures are listed in Table 1 below.

We have selected the silicon and polystyrene materials to ensure large refractive index contrast which is a prerequisite for getting large PBG. Moreover, these materials have very low absorption in the region of investigation. The refractive
index values of various EV samples used as an analyte in this study are listed in Table 2.

The total number of the periods (N) of structure (AB)^N are taken as 8. The thickness of defect layer C is to be 109 nm in both structures.

### 3.2 Numerical results

First we investigate the transmission spectra of conventional 1D photonic structure (AB)^8 under normal incidence as shown in Fig. 2. Figure 2 shows the transmission spectra of a periodic 1D PC with wide PBG in visible region of electromagnetic spectrum extending from 493.6 nm to 764.5 nm which is similar to the findings of Wu and Wang for symmetric 1D PCs [37]. In this range of PBG, almost zero transmission has been noticed and hence PBG is said to be complete as shown in Fig. 2. Next we split the structure (AB)^8 in two sub identical PC structures as (AB)^4. The cavity region C of thickness d_c = 109 nm is sandwiched between two sub identical PCs to form a 1D defective photonic structure (AB)^4C(AB)^4. Here, we have taken 100% distilled water solution of refractive index 1.333 as an external reference inside the cavity region C. The break in periodicity due to the defect layer C results a defect mode of intensity more than 92% located at 586.7 nm inside the PBG (Fig. 3). This defect layer C can be treated as an equivalent to Fabry–Perot cavity between two identical cavity walls (AB)^4. The electromagnetic radiations which satisfy the resonance condition 2n_d d_c = mλ_d, m = 1, 2, 3, ... will suffer series of reflections and transmissions inside the cavity region which results localization of electromagnetic waves inside cavity region. The energy associated due to this localization of electromagnetic radiation will come out from laser cavity in the form of defect mode of almost 92% transmission inside PBG of a 1D defective photonic structure (AB)^4C(AB)^4 loaded with sample of distilled water as shown in Fig. 3. The various EV samples which are under investigation will be poured one by one for sensing into the cavity region with the help of opening embedded into the upper surface of the structure as shown in Fig. 1b. Thus, the cavity reason can be used as an important sensing tool by infiltrating various EV samples into it. The above findings are similar to the results proposed by Aly et. al. [19, 20, 23]

Next the efforts have been made to improve the sensing capabilities of the proposed sensor consisting of single defect as discussed above. For this purpose, we have modified the aforementioned photonic structure (AB)^4C(AB)^4 by inserting two identical defect layers C side by side in the middle of the structure (AB)^8. The transmission spectra of this modified structure (AB)^4CC(AB)^4 containing two identical defect layers of 100% distilled water of refractive index 1.333 and thickness 109 nm each, are shown in Fig. 4. Due to break in periodicity a defect mode of unit transmission, located at 715.2 nm is found inside PBG as shown in Fig. 4. The reason behind the existence of this defect mode of unit transmission inside PBG is also due to Fabry–Perot
This structure is assumed to have Fabry–Perot cavity between mirror image cavity walls due to sub PCs $(AB)^4$ and $(BA)^4$ which offer reflection phase of 0 and $\pi$, respectively, at interfaces contrary to nature of the cavity of photonic structure $(AB)^4C(AB)^4$ [25, 36] (Figs. 5 and 6).
Fig. 5 Transmission spectra of proposed 1D defective PC (AB)₄C(AB)₄ as a function of incident wavelength at normal incidence. Here 100% distilled water has been taken as an external reference along with seven EV samples separately in place of defect layer C of thickness 109 nm.

Fig. 6 Extended portion of transmission spectra of proposed 1D defective PC (AB)₄C(AB)₄ as a function of incident wavelength shown in Fig. 5 to make all defect modes corresponding to various samples clear and distinct.
3.3 Comparison between 1D defective PCs consisting of single and double defect layers for sensing of various EV samples

Now we examine the sensing capabilities of both 1D defective photonic structures (AB)\(^4\)C(AB)\(^4\) and (AB)\(^4\)CC(BA)\(^4\). For this purpose, we have loaded both structures with various EV samples one by one under consideration as per the data given in Table 2 by replacing the distilled water solution with different EV samples through the opening which is embedded on the top surface of the both structures as shown in Fig. 1b and c. Transmission spectra of both structures loaded with various EV samples in addition to distilled water sample are plotted in Figs. 5 and 7, respectively. Both the figures show that the increase in the refractive index of various EV samples with respect to the refractive index of distilled water solution results red shift in the central wavelength of respective defect modes. The comparison between transmission response of structures (AB)\(^4\)C(AB)\(^4\) and (AB)\(^4\)CC(BA)\(^4\) shows that the presence of mirror image cavity walls in structure (AB)\(^4\)CC(BA)\(^4\), significantly enhanced the intensity of transmission peaks of defect modes (Figs. 5 and 7). Besides this the photonic structure (AB)\(^4\)CC(BA)\(^4\) also reduces the full width half maxima (FWHM) of transmission peak of defect mode associated with each sensing sample as evident from Figs. 6 and 8. This reduction in FWHM of defect mode improves the quality (Q) factor and figure of merit (FOM) of the structure which is one of the essential requirements for the better performance of the photonic biosensing designs. Thus, the double defect photonic structures with mirror image cavity walls can serve as a better alternative for designing of highly sensitive sensors of larger Q and FOM values.

3.4 Analysis of the sensing performance of proposed photonic structures

Under the choice of structural parameters as described above, efforts have been made to analyze the performance of photonic sensor designs (AB)\(^4\)C(AB)\(^4\) and (AB)\(^4\)CC(BA)\(^4\) which are capable of sensing the various EV samples to determine their refractive index based on their size and counts. The linear curve fitting between the refractive index of various EV samples and corresponding wavelength of the defect modes are plotted in Fig. 9 for structure (AB)\(^4\)C(AB)\(^4\). The slope of linear curve fitting data determines the average value of sensitivity 113.92 nm per RIU of one of our proposed design (AB)\(^4\)C(AB)\(^4\) as per the following equation:

\[
\lambda_C = 113.92n_C + 434.83, \quad (R^2 = 0.9998) \tag{6}
\]

Here \(\lambda_C\) is the central wavelength of defect mode in nm corresponding to refractive index \(n_C\) of EV sample. The square of the correlation coefficient \(R\) between linear curve fitting and theoretical data is 0.9998 which is close to one. The high value of \(R^2\) indicates that the sensitivity of biosensor is very

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Fig. 7: Transmission spectra of proposed 1D defective PC (AB)\(^4\)CC(BA)\(^4\) as a function of incident wavelength at normal incidence. Here 100% distilled water has been taken as an external reference along with seven EV samples separately in place of both defect layer C each of thickness 109 nm.
Fig. 8 Extended portion of transmission spectra of proposed 1D defective PC (AB)4C(AB)4 as a function of incident wavelength shown in Fig. 7 to make all defect modes corresponding to various samples clear and distinct.

Fig. 9 Linear curve fitting relation between refractive index of various EV samples and the positions of their respective defect modes of structure (AB)4C(AB)4.
high. Usually for analyzing the efficiency and performance of any biosensor we use sensitivity ($S$), quality factor ($Q$) figure of merit (FOM) and limit of detection (LOD) values as describe below

$$S = \frac{\Delta \lambda C}{\Delta n C}$$  
(7)

Here the refractive index of distilled water is 1.333 and its respective defect mode of central wavelength 586.7 nm are taken as reference to evaluate $\Delta \lambda C$ and $\Delta n C$ of various EV samples under consideration, i.e., $\Delta \lambda C = \lambda C$ (corresponding to various EV samples) − 586.7 (corresponding to distilled water sample) and $\Delta n C = n C$ (refractive index of various EV samples) − 1.333 (refractive index of distilled water set as reference).

The higher value of FOM specifies a larger sensitivity and smaller value of FWHM of resonant peak. For high performance sensors a larger value of FOM is always expected. FOM is defined as

$$FOM = \frac{S}{\lambda _{FWHM}}$$  
(8)

The ability of any sensor having narrow bandwidth is determined by $Q$ factor. Higher $Q$ value is always expected. It is defined as

$$Q = \frac{\lambda C}{\lambda _{FWHM}}$$  
(9)

Finally, the smallest detectable change in refractive index noticed by sensor is determined by LOD as defined below

$$LOD = \frac{\lambda C}{20 \times S \times Q}$$  
(10)

Table 3 summarizes the $S$, $Q$ factor, FOM and LOD values of one of the proposed design (AB)$^4$C(AB)$^4$ loaded with different EV samples. It is evident from Table 3 that the design (AB)$^4$C(AB)$^4$ has an average sensitivity of 113.92 nm per RIU, figure of merit variations are between 6.98 $\times$ 10$^2$ RIU to 7.75 $\times$ 10$^2$ RIU and $Q$ factor variations are between 3.91 $\times$ 10$^3$ to 3.97 $\times$ 10$^3$ which is comparable to the $Q$ values of the photonic structure design based refractive index gas sensor proposed by Ahmed et. al. The LOD values of one of our proposed structure (AB)$^4$C(AB)$^4$ vary between 7.16 $\times$ 10$^{-5}$ and 6.60 $\times$ 10$^{-5}$.

Finally $S$, $Q$ factor, FOM and LOD values of our mirror image design (AB)$^4$CC(BA)$^4$ loaded with different EV samples are summarized in Table 4.

| Sample description       | $n_c$ | $\lambda_c$ (nm) | $S$ (nm/RIU) | $\chi_{FWHM}$ (nm) | $Q$ factor | FOM (per RIU) | LOD RIU |
|--------------------------|-------|------------------|---------------|--------------------|------------|---------------|---------|
| Distilled water          | 1.333 | 584.9            | 0.07          | 8355.71            |
| Lyophilized urinary EV   | 1.367 | 589.6            | 0.07          | 8422.86            | 1974.79    | 2.53E-05      |
| Fresh urinary EV         | 1.374 | 590.5            | 0.07          | 8435.71            | 1951.22    | 2.56E-05      |
| Small placental EV       | 1.375 | 590.7            | 0.07          | 8438.57            | 1972.79    | 2.53E-05      |
| Activated platelets EV   | 1.39  | 592.8            | 0.07          | 8468.57            | 1979.95    | 2.53E-05      |
| Neuroblastoma EV         | 1.393 | 593.3            | 0.07          | 8475.71            | 2000.00    | 2.50E-05      |
| Blood EV                 | 1.398 | 594              | 0.07          | 8485.71            | 2000.00    | 2.50E-05      |
| Large placental EV       | 1.414 | 596.3            | 0.07          | 8518.57            | 2010.58    | 2.49E-05      |

Table 4 Various parameters of proposed photonic biosensor (AB)$^4$CC(BA)$^4$ at optimum conditions

| Sample description       | $n_c$ | $\lambda_c$ (nm) | $S$ (nm/RIU) | $\chi_{FWHM}$ (nm) | $Q$ factor | FOM (per RIU) | LOD RIU |
|--------------------------|-------|------------------|---------------|--------------------|------------|---------------|---------|
| Distilled water          | 1.333 | 584.9            | 0.07          | 8355.71            |
| Lyophilized urinary EV   | 1.367 | 589.6            | 0.07          | 8422.86            | 1974.79    | 2.53E-05      |
| Fresh urinary EV         | 1.374 | 590.5            | 0.07          | 8435.71            | 1951.22    | 2.56E-05      |
| Small placental EV       | 1.375 | 590.7            | 0.07          | 8438.57            | 1972.79    | 2.53E-05      |
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| Neuroblastoma EV         | 1.393 | 593.3            | 0.07          | 8475.71            | 2000.00    | 2.50E-05      |
| Blood EV                 | 1.398 | 594              | 0.07          | 8485.71            | 2000.00    | 2.50E-05      |
| Large placental EV       | 1.414 | 596.3            | 0.07          | 8518.57            | 2010.58    | 2.49E-05      |
It has been found the mirror image design improves the sensitivity as well as reduced the FWHM of defect mode. This reduction in FWHM results the significant improvement in FOM and Q values of this mirror image design which are between 1974.79 per RIU to 2010.58 per RIU and 8355.71 to 8518.57, respectively. The order of LOD values of mirror image design \((AB)^4CC(BA)^4\) is \(10^{-5}\) similar to that of structure \((AB)^4C(AB)^4\) as discussed above. The linear curve fitting between the refractive index of various EV samples and corresponding wavelength of their defect modes are plotted in Fig. 10 for structure \((AB)^4CC(BA)^4\). The slope of linear curve fitting data determines the average value of sensitivity of 140.81 nm per RIU of one of our proposed design \((AB)^4CC(BA)^4\) as per the following equation:

\[
\lambda_C = 140.81n_C + 397.12, \quad (R^2 = 0.9998)
\]  

(11)

The square of the correlation coefficient \(R\) between linear curve fitting and theoretical data is high which indicates that the mirror image photonics structure design \((AB)^4CC(BA)^4\) also have high sensitivity values similar to the finding discussed above for the structure \((AB)^4C(AB)^4\) [38].

Thus by sensing and detecting the position of defect mode depending upon the various EV samples one can easily estimate the refractive index of various EV samples. For this purpose, we have to compare the results of proposed work with the standard experimentally available data similar to that of Table 2. The proposed findings based on present photonic technology may also be helpful to find refractive index of various EVs. This is very difficult by available conventional optical technologies because most of EVs have their diameter smaller than the wavelength of the light in visible region so could not be resolved by means of light microscopy.

4 Conclusion

In summary, we have theoretically investigated how refractive index as well as size and count of extracellular vesicles can be detected from various EV samples. For this purpose, we have used 1D defective PC based sensing technique. The various EV samples have to be injected into cavity region one by one in both the structures and the corresponding shift in defect mode inside the PBG is measured. Thus by knowing the shift in position of the defect mode required information about various EV samples can be retrieved, for this purpose we have to compare these observations with the experimentally available data which is not possible by using conventional optical techniques because most of EVs have their diameter smaller than the wavelength of the light in visible region. Beside this we have also explored how mirror image defect structure consisting of 1D defective planar PC
designs can be used as a biosensor as an alternative of 1D APC without defect with air core in which propagation of electromagnetic waves is along the radial direction. Furthermore, we have compared the conventional and mirror image 1D defective PC designs and found that the mirror image structure can be used to get narrow transmission peak of unit transmission inside the PBG. Thus, mirror image based photonic sensing designs have higher sensitivity, larger FOM & Q values and lower LOD value which are essential for any high performance biosensors.

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**Code availability**  No code has been used.

**Declarations**

**Conflicts of interest**  Authors have declared that there is no conflict of interest.

**Consent to participate**  Author consent was obtained from all individual participants included in the study.

**Consent for publication**  Author consent was obtained from all individual participants to publish in this journal.

**Ethical approval**  This article does not contain any studies with human participants performed by any of the authors.

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