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One Dimensional Photonic Crystal with Defects for Detecting Lard Oil Chemical Substances: Theoretical Approach

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ABSTRACT

Adulteration and mixing food with ingredients that do not meet health standards and religious teachings have caused great concern among consumers. Mixing food and pharmaceutical products with cheaper raw materials has become common. One of the most common adulterations in food and pharmaceuticals is the use of lard substances. In this paper we focus on the theoretical modelling and simulation of identifying lard oil characteristics using 1D photonic crystal (PhC) with defects. The presence of lard oil in the defect layer of 1D PhC altered the transmission spectrum. The proposed 1D PhC structure consists of air/$(Ta_2O_5/SiO_2)^N$/defect/$(Ta_2O_5/SiO_2)^N$/air with a defect layer consisting lard oil placed in the middle. To calculate the transmittance and reflectance characteristics of 1D PhC, the MATLAB software has been used based on transfer matrix method (TMM). We have considered the normal light incident to PhC to eliminate the difficulties with the oblique incident in the visible light spectrum. Various sensor parameters, such as sensitivity (*S*), quality factor (*Q*), figure of merit (*FOM*), resolution (*RS*) and detection limit (*LOD*) have been calculated to evaluate sensor performances. The average *S* of this structure is 212.319 nm/RIU, the average *Q* value is 779.45, the average *FOM* value is 249.78, and the average *LOD* is 0.0002012. These values show that our simple design could be a promising non-invasive detection method, with potential applications in the food and pharmaceutical industries for monitoring and identifying non-halal and non-kosher substances.

1. Introduction

Food and pharmaceutical products are very important for human needs. The high demand for products due to the increased population and supported by current conditions of globalization, new industries, and the advancement of technology have triggered pressure on the industry to fulfill the needs [1]. The technological progress supporting industrial growth has also generated various new products manufactured for wider needs. However, technological advances in the industrial sector have triggered fraud in the food and pharmaceutical industry, creating concern for many societies [2][3]. The fraud may contain food ingredients that do not meet the needs of some communities,

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such as Muslim, and Jewish. This is a major issue because the basic materials used as ingredients and the production process may need to meet the needs of the religious beliefs of some people who use them [4]. One food ingredient often found in food and pharmaceutical products is lard [5][6].

Lard extracted from pig adipose tissues is a good substitute for expensive oil and fats in the food and pharmaceutical industry [7]. In food and pharmaceutical commodities, lard is mixed with other oils, such as vegetable oils, to make margarine, shortening, and other foods and pharmaceutical products based on fats and oils. However, lard is forbidden to be consumed by Muslims and Jews, because of religious restraint. Therefore, detecting lard in food and pharmaceutical goods becomes extremely urgent to ensure it complies with halal and kosher rules [8][9].

Currently, several detection methods have been used to detect food and pharmaceutical stuffs by lard adulteration, such as Fourier transform infrared spectroscopy (FTIR), DNA-based polymerase chain reaction(PCR), electronic nose technology (e-nose), high-performance liquid chromatography (HPLC), differential scanning calorimetry (DSC), etc. However, apart from their accuracy and widespread use, most of these methods have disadvantages such as being unsuccessful in food and pharmaceutical products, only suitable for certain solution sources, and the spectra being too complex, time-consuming, and high cost [10]. To overcome such shortcomings, in this paper, we proposed using PhC as a biosensor to detect lard oil substances.

PhC has gained substantial attention recently for its unique ability to manipulate and control light flow through precisely engineered periodic structures. These materials exhibit photonic bandgaps, regions where specific wavelengths of light are forbidden to propagate, making them highly valuable for a wide range of optical applications. Among the various types of photonic crystals, one-dimensional (1D) photonic crystals offer the advantages of simple design, ease of fabrication, and high tunability, which make them suitable for practical applications in optical sensing. [11]-[13].

1D PhCs are smart materials created by arranging dielectric structures in a multilayer periodic pattern, defined by their refractive index constants. This arrangement gives PhCs the distinctive capability to regulate the transmission of electromagnetic waves. Periodic structures give rise to photonic bandgaps (PBGs), certain frequency ranges between which light cannot pass through the crystal [14]. PhC exhibits a particularly intriguing characteristic in their reaction to faults. When defects are deliberately introduced to disturb the periodicity, they generate localized modes inside the photonic bandgap. The presence of these defect modes enables the transmission of selected wavelengths of light through otherwise reflecting structure, generating highly localized wavelength resonances. Modifications in the dielectric environment surrounding the defect can affect the wavelength of these localized modes. Small fluctuations in the refractive index, caused by the existence of a chemical or biological agent, might cause a change in the defect mode. This makes photonic crystals suitable for highly sensitive sensing applications [15]-[26].

This paper explores the potential application of 1D PhC with a defect layer to detect lard oil. Introducing a defect layer within the periodic structure of the photonic crystal breaks the symmetry and introduces localized defect modes within the photonic bandgap. These defect modes are highly sensitive to changes in the refractive index of the materials within the defect region, making the system an excellent candidate for lard sensing applications.

2. Methodology

2.1 ***One-Dimensional Photonic Crystals: Theory***

The proposed 1D PhC capable of detecting lard oil via its refractive index characteristics is shown in Fig. 1. The 1D photonic crystal used in this study is constructed with alternating layers of two dielectric materials, Ta_2O_5 and SiO_2, selected for their contrasting refractive indices and ease of

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fabrication. The structure is designed as air/$(Ta_2O_5/SiO_2)^N$/defect/$(Ta_2O_5/SiO_2)^N$/air, where N represents the number of periods. Different colors in the diagram correspond to various layers of the structure, with thicknesses denoted as d_1, d_2 and the defect layer thickness d_c, respectively. A defect layer is inserted at the center of the structure. The purpose of introducing the defect cavity is to allow for the insertion of various samples for investigation. The thickness layers were defined by Bragg's law, considering that the photonic bandgap will appear around the wavelength, which describes the maximum constructive interference in its strongest form. By assuming that the incoming light is in a normal incident, the defect thickness can be defined as follows [27]:

$$d_j = \frac{\lambda_o}{4n_j} \tag{1}$$

Where j is the j^{th} layers, and λ_o is the Bragg wavelength. The defects width use is defined as $d_c = d_1 + d_2$. The number of layers and the thicknesses are optimized to produce a well-defined photonic bandgap in the desired wavelength range. A combination of the transfer matrix method and MATLAB software computational tools was used to simulate the transmission and reflections of the PhC structure. MATLAB is the most suitable technique for the computation and simulation of the proposed 1D PhC, as shown in Figure 1. The TE mode can be calculated using the continuity condition at the interface layer of different materials. The mathematical relation can be expressed in a matrix, which correlates the field on each side of the layer. Then, the amplitude of transmitted and reflected wave at the end of the PhC structures can be defined in a complete matrix as a multiplying all individual matrices and given by [28]-[32]:

$$M = (m_1 m_2)^N m_{d_c} (m_2 m_1)^N = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \tag{2}$$

M_{11}, M_{12}, M_{21}, and M_{22} are the matrix element of resultant matrix M. The m_1, m_2, and m_{d_c} represent the matrix characteristics of A, B, and defect layers, respectively. The transfer matrix representing the j layer of the proposed design is given by [28]:

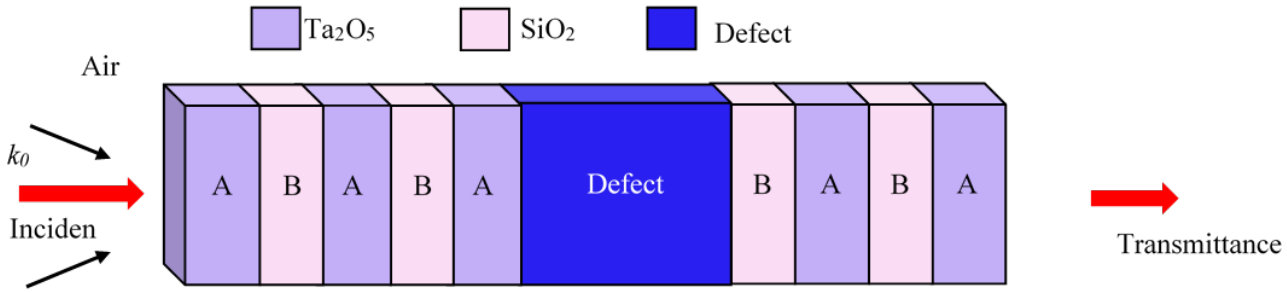


Figure. 1. Proposed design of 1D PhC with defect capable of detecting lard oil

$$M_j = \begin{bmatrix} \cos k_j & \frac{i \sin k_j}{p_j} \\ -ip_j \sin k_j & \cos k_j \end{bmatrix} \tag{3}$$

Where $k_j = \frac{2\pi n_j d_j}{\lambda}$, in this case, n_j is the refractive index of the j^{th} layer, d_j is the width of the j^{th} layer, and λ is the wavelength. The transmission and reflection coefficients for the proposed design might be defined as [27]:

$$r = \frac{M_{21}}{M_{11}}, t = \frac{1}{M_{11}} \tag{4}$$

Hence, the reflectance (R) and transmittance (T) of the structure can be calculated as [27]:

$$R = |r|^2 = \left|\frac{M_{21}}{M_{11}}\right|^2, T = |t|^2 = \left|\frac{1}{M_{11}}\right|^2 \tag{5}$$

Several biosensor performances have been used to evaluate the effectiveness of proposed PhC structures. Below are some parameters used in the calculation and their definitions and equations.

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The sensitivity (*S*) is defined as the ratio of resonance peak change to the change in refractive index and can be calculated by using the following Equation which are taken from previous study [31]-[34]:

$$S = \frac{\Delta\lambda_R}{\Delta n_{Lard}} \quad (6)$$

Here $\Delta\lambda_R$ is the resonance peak change, and Δn_{Lard} is the refractive index change relative to the lowest refractive index of lard oil and measured in nm/RIU. Additionally, the quality factor (*Q*), which describes the resonant peak sharpness, is defined as the ratio of resonance wavelength at each different refractive index to the transmittance full wave half width maximum (*FWHM*) signals and can be calculated by the following relation:

$$Q = \frac{\lambda_R}{FWHM}. \quad (7)$$

Figure of merits (*FOM*) is the measure of the ability of the sensors to analyze the change of resonance peak; it is defined as the ratio between the sensitivity and the FWHM of the resonant peaks and can be calculated as follows:

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

The resolution (*RS*) is defined as a small central wavelength change of defect modes and is given by:

$$RS = \frac{2(FWHM)}{3SNR^{\frac{1}{4}}} \quad (9)$$

The dynamic range (*DR*) is the range of sample refractive index that can produce reliable refractive index change and is given as follows:

$$DR = \frac{\lambda_R}{\sqrt{FWHM}} \quad (10)$$

3. Results and Discussion

This simulation calculates the transmittance along the light spectrum range of 400-900 nm using MATLAB software based on TMM. The incoming wave is assumed to be a normal incident to eliminate the difficulties with the oblique incident. The Ta_2O_5 and SiO_2 refractive index are 2.1224 and 1.4573, respectively, and *N*=5 periods. The material used in the PhC structure is assumed to be homogeneous, isotropic, and non-magnetic [15]. The Ta_2O_5 and SiO_2 widths are calculated using Equation 1 with the reference wavelength of λ=623 nm. The chemical and physical characteristics of lard oil refractive index at 40°C range from 1.448 to 1.460 [35]. In this calculation, a refractive index increase of 0.002 has been used. Fig. 2 demonstrates the transmittance spectrum for PhC as a function of wavelength without defects, a well-defined photonic crystal bandgap with 105.55 nm spectral width.

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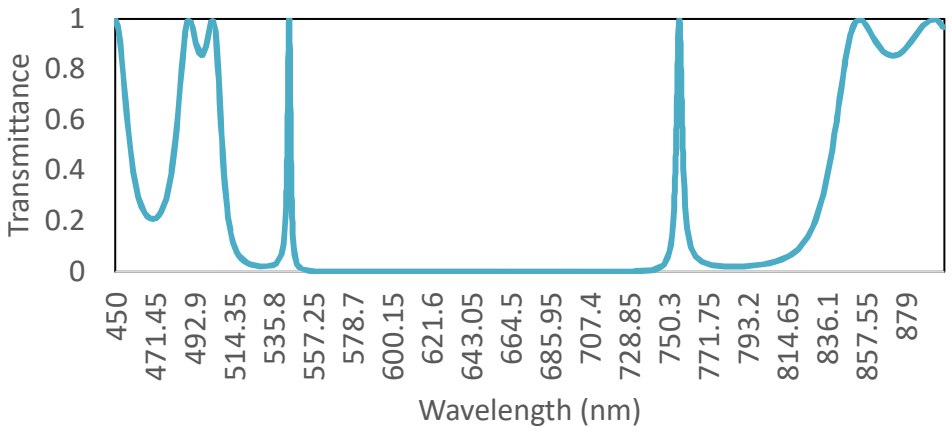


Figure. 2. Transmittance as a function of wavelength without defects

Fig. 3 compares the proposed PhC's transmittance spectrum with a defect refractive index of 1.450 and 1.460, respectively. When a defect layer is inserted at the center of the PhC, the spectral width increases to 148.9 nm. Figure 3 also shows a comparison of the resonance peaks between lard oil with a refractive index of 1.448 (λ_P= 661.19 nm) and 1.460 (λ_P=663.55 nm). It can be observed that the resonance peak shifts by 2.36 nm.

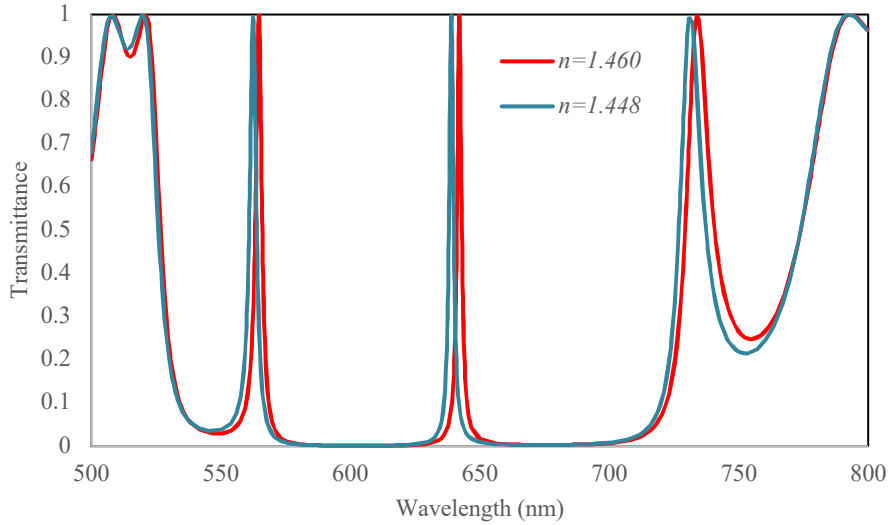


Figure 3. Transmittance as a function of wavelength for PhC with defect containing lard oil

Fig. 4 shows the transmission spectra of 1D PhC when the defect layers are loaded with different lard oil refractive indices. The defect resonance wavelength starts to shift toward higher wavelength values due to the increase in the refractive index of lard oil. The amplitude intensity of each different refractive index is almost unity, enough to be detected by the transducer for the proposed PhC design. The full half-width maximum of resonance wavelength is constant at 0.85 nm, which is also an essential requirement for a good quality biosensor design.

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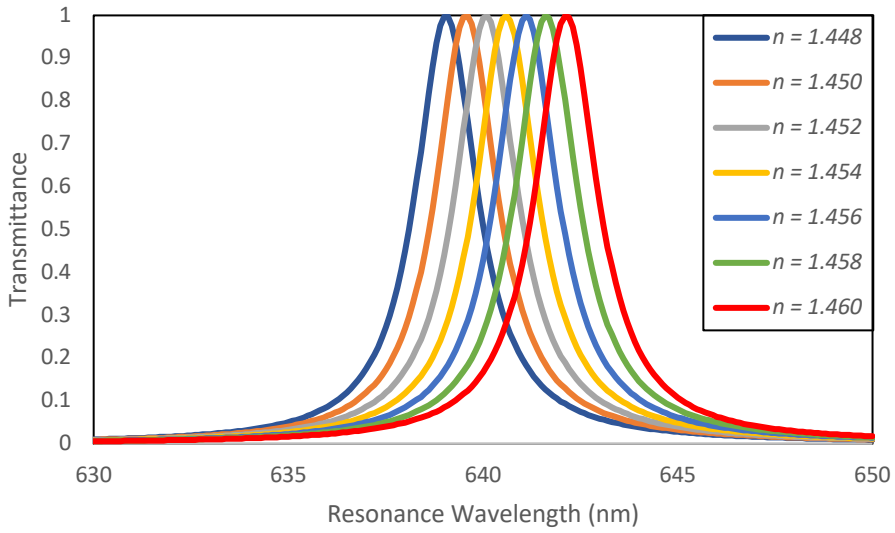


Figure. 4. Transmittance is a function of resonance wavelength shift with different lard oil refractive indexes.

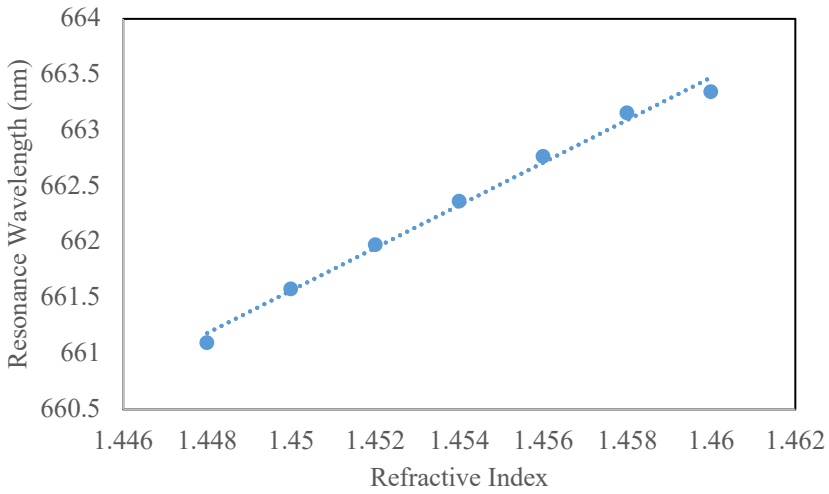


Figure. 5. Resonance wavelength shift as a function of refractive index change.

Fig. 5 illustrates the resonance wavelength as a lard oil refractive index function. The resonance wavelength shift varies linearly with the refractive index, and the relation can be found using least square fitting and expressed in the following Equation.

$$RW = 191.07\ RI + 384.51 \quad (12)$$

RW is the Resonance Wavelength, and *RI* is the lard oil refractive index.

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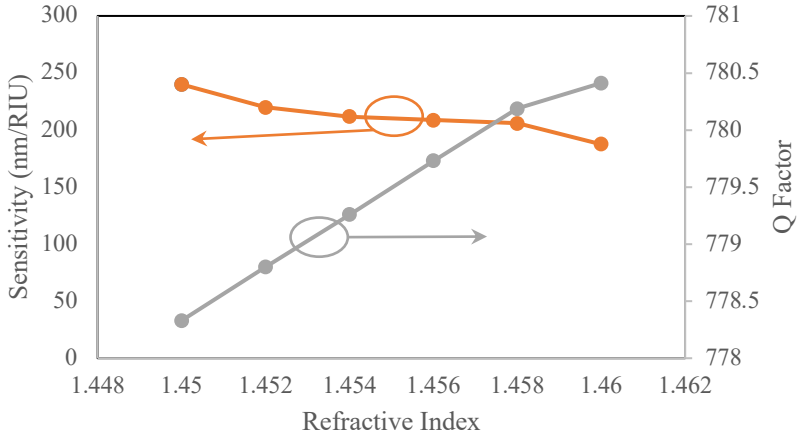


Fig. 6. Variation of sensitivity and *Q* factor as a function of the refractive index change

Fig. 6 demonstrates the sensitivity and *Q* factor dependence to the change of lard oil refractive index. In a 1D photonic crystal (PhC) with a defect layer, the relationship between the sensitivity and *Q* factor is fundamental to understanding how the photonic crystal behaves when subjected to changes in its environment, particularly the refractive index or other physical properties. A high *Q* factor indicates a very sharp resonance. When the resonance is sharp, the energy is highly confined within the defect mode, meaning that the interaction between the defect mode and the surrounding medium is minimized. As a result, small changes in the refractive index or other properties of the surrounding medium will cause only a small shift in the resonance wavelength. Thus, the system becomes **less sensitive** to changes in the environment. The sharpness of the resonance peak implies that the defect mode is highly localized, with minimal energy leakage into the surrounding medium. This confinement reduces the interaction between the mode and the external environment, making it **less responsive** to small perturbations, leading to **lower sensitivity**. A lower *Q* factor corresponds to a broader resonance peak. In this case, the energy is less tightly confined in the defect mode, and the mode interacts more with the surrounding medium. When the refractive index of the surrounding medium changes, the broader resonance allows for a more significant shift in the resonance frequency. This results in higher sensitivity, as the system responds more strongly to changes in the environment. A lower *Q* factor means that the defect mode is more easily perturbed by external changes. The broader resonance peak indicates that the defect mode is less selective and more influenced by the surrounding medium, which increases the **sensitivity** to changes in environmental conditions. For applications like chemical or biological sensing, **higher sensitivity** is often desired to detect small changes in the refractive index of the surrounding medium. In this case, a lower *Q* factor might be preferred, as it allows for more significant shifts in the resonance frequency in response to environmental changes.

Figure 7 demonstrates the resonance wavelength as a function of defect width. As the defect layer's width changes, the resonance wavelength of the defect mode shifts. The defect layer essentially creates a resonant cavity within the photonic crystal. The width of this defect cavity plays a crucial role in determining the wavelength at which the system resonates. When the defect layer becomes wider, the localized mode has more space to resonate This results in a **longer resonance wavelength**. From a physical perspective, a wider defect provides a larger cavity, which allows the resonance mode to have a longer period (longer wavelength).

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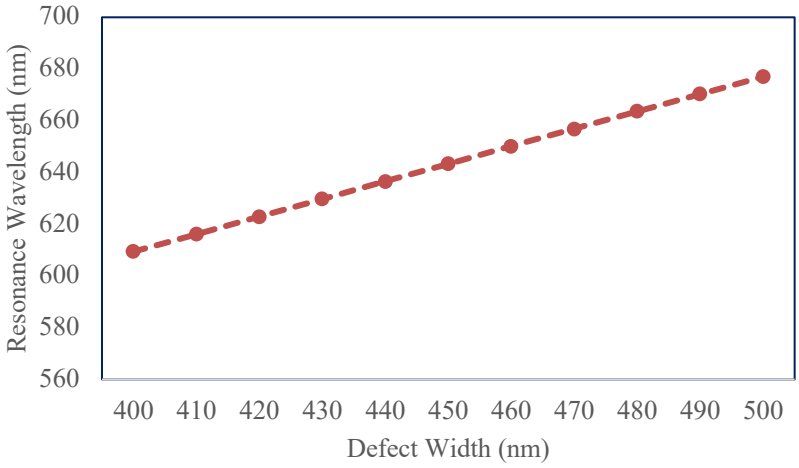


Fig. 7. Resonance wavelength as a function of defect width

Table 1 summarizes the calculation parameters, including Sensitivity, *Q* factors, *FOM*, *RS*, and *LOD*.

Refractive Index	λ_R (nm)	*S* (nm/RIU)	*Q*	*FOM*	*RS*	*LOD*
1.448	661.1					
1.45	661.58	240.000	778.329	282.353	0.650	0.000177083
1.452	661.98	220.000	778.800	258.824	0.562	0.000193182
1.454	662.37	211.667	779.259	249.020	0.515	0.000200787
1.456	662.77	208.750	779.729	245.588	0.482	0.000203593
1.458	663.16	206.000	780.188	242.353	0.458	0.000206311
1.46	663.35	187.500	780.412	220.588	0.449	0.000226667

Table 1 presents the numerical values of sensitivity (*S*), quality factor (*Q*), figure of merit (*FOM*), resonance shift (*RS*), and limit of detection (*LOD*) for various refractive indices. The full width at half maximum (*FWHM*) of the defect mode remains consistently narrow across the entire refractive index range, which is a critical factor in achieving high sensitivity. The sensitivity of the proposed sensor ranges from 187 nm/RIU to 240 nm/RIU, depending on the refractive index of the material filling the defect layers. The average Q-factor and FOM are calculated to be 779.45 and 249.78, respectively. Additionally, the average RS and LOD are determined to be 0.519 and 0.0002012, respectively. The low LOD values indicate the sensor's capability to detect changes in refractive index with high precision. These results suggest that the proposed photonic structure is well-suited for the effective detection of lard oil variations within the specified refractive index range.

4. Conclusion

We have demonstrated the biosensor performances of 1D photonic crystal with defects to detect the lard oil substance. We used the transfer matrix methods for numerical analysis of transmittance spectra using MATLAB software with normal light incident to PhC with varying lard oil refractive index. The sensor consists of air/$(Ta_2O_5/SiO_2)^N$/defect/$(Ta_2O_5/SiO_2)^N$/air. The sensor performances have been analyzed by calculating the sensitivity, quality factor, figure of merit, resolution, and dynamic range. The simulation only considers detecting lard oil within the range of refractive index changes. The empirical formulae deducted from this simulation to estimate the resonance

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wavelength shift due to refractive index change can be used to estimate the resonance wavelength shift caused by lard oil. We believe the proposed biosensor is very useful for detecting food and pharmaceutical product adulteration of lard oil. The proposed sensor structure is very simple and easy to fabricate.

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