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Modeling and Simulation of Photonic Crystal Sensor for Drinking Water Quality Monitoring

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ABSTRACT: Photonics crystal sensors, sensitive to light, play a crucial role in discerning minute alterations in a material's refractive index, finding widespread application, such as in monitoring drinking water quality. Our objective is to fashion a sensor based on a 2D photonics crystal structure and scrutinize optical transformations induced by variations in the bacteria's refractive index as light traverses the sensor structure. Leveraging Rsoft's simulation capabilities, we assessed transmission spectra, observing shifts in the bacteria's refractive index and their consequential impact on the light signal's frequency and wavelength within the sensor structure. The simulations unequivocally demonstrate that fluctuations in the bacteria's refractive index significantly affect the light signal's frequency and wavelength. Consequently, the study underscores the efficacy of the Rsoft-designed optical sensor in discerning bacterial presence in contaminated water, achieving an average sensitivity of 834.344 nm/RIU. In conclusion, the study establishes the success of the optical sensor crafted with Rsoft software in detecting bacteria in polluted water. By monitoring optical alterations during light traversal, variations in the bacteria's refractive index are translated into discernible shifts in the light signal's frequency and wavelength, facilitating effective bacteria detection.

1. INTRODUCTION

Water quality is a major global concern with direct implications for public health and the environment. Traditional methods of monitoring water purity are limited in terms of sensitivity and speed, emphasizing the need for more advanced technologies. Current challenges related to water contamination demand sophisticated detection solutions due to potential risks to human health and biodiversity. The development of a photonic crystal sensor for water purity detection is motivated by the need to overcome these limitations, providing real-time detection, increased sensitivity, and selectivity for specific contaminants. Improving water quality monitoring is crucial for public health and the preservation of aquatic ecosystems. This innovative sensor aims to contribute to more effective water resource management and prevent environmental risks. In the current context of growing concerns about water safety, this study on photonic crystal sensors represents a significant advancement, offering extensive application prospects in the fields of public health, environmental management, and water resource sustainability. This study proposes an innovative solution to address urgent challenges related to water quality, with the potential to have a lasting impact on the preservation of our vital water resource. Photonic crystals, these nanostructures with exceptional optical characteristics, have revolutionized the field of optics by enabling precise manipulation of light on a nanoscale level. These crystals exhibit a periodic arrangement of dielectric materials, creating photonic bandgaps that prevent the propagation of certain wavelengths of light. Thanks to these properties, they have paved the way for a range of innovative applications, from high-speed optical communication to ultra-sensitive sensors [1–8].

Photonic crystal sensors, sophisticated detection tools, utilize these properties to monitor subtle environmental changes. Interactions with particles, molecules, or microorganisms alter the local electromagnetic field, causing variations in the crystal's optical properties. This technology offers exceptional sensitivity, facilitating precise real-time detection of specific elements like bacteria in water [9].

Indicator bacteria are microorganisms that serve as alarm signals during analyses aimed at detecting the contamination of drinking water. When such bacteria are present in the water we consume, it can have various impacts on health, ranging from the absence of symptoms to severe gastrointestinal disorders. Gastrointestinal symptoms can manifest after a certain period, ranging from a few hours to several weeks after ingestion, and may include nausea, vomiting, abdominal cramps, diarrhea, muscle aches, headaches, and mild fever. In exceptional cases, the consumption of contaminated water can even lead to serious illnesses, or even death [10].

It is important to note that anyone can become ill from drinking contaminated water, but children, the elderly, and those with weakened immune systems are more susceptible to the adverse effects of contamination [11].

Total coliforms and Escherichia coli (E. coli) are types of bacteria used as indicators, often referred to as target bacteria, to assess the quality of drinking water. On the other hand, other bacteria that may be present in drinking water are considered non-target bacteria. The sanitary quality of water is evaluated based on the concentration of target bacteria detected in water samples [12–15].

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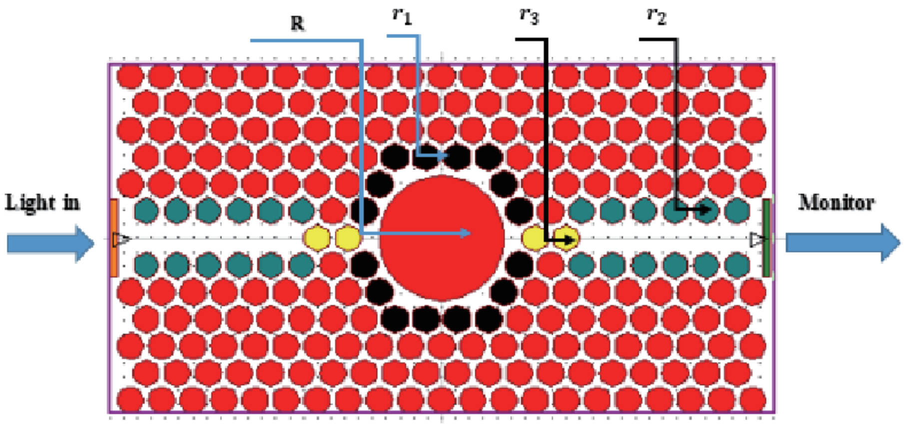

FIGURE 1. Schematic of the proposed 2D-PhC biosensor.

The rapid and accurate detection of bacteria in contaminated water is crucial for public health preservation and environmental management. Pathogenic bacteria, such as E. coli and Salmonella, can lead to outbreaks of severe and sometimes deadly gastrointestinal diseases. Furthermore, bacterial contamination can compromise the quality of water intended for human consumption, agriculture, and industry [16–18].

In the quest for bacterial detection, technological advancements have led to the emergence of optical photonic crystal sensors as promising tools. These sensors exploit the optical properties of photonic crystals to detect changes in refractive index caused by the presence of bacteria in water. When bacteria are within the sensor's detection field, they alter the refractive index of the medium, thereby causing characteristic changes in the properties of the light passing through the photonic crystal.

This innovative approach opens up fascinating prospects for the rapid and sensitive detection of bacteria in water. In this article, we will explore recent advances in the field of bacterial detection using photonic crystal sensors. We will analyze the operating principles of these sensors, the design method. Additionally, we will examine how these devices can contribute to addressing crucial challenges related to water safety and public health [19].

In this context, a highly sensitive 2D refractive index sensor based on Photonic Crystals (PhCs) has been developed and introduced for the detection of bacteria in water. The novel PhC biosensor comprises two waveguides coupled with a single defective circular-shaped microcavity. To create the central cavity, every seventh hole in the lattice structure was intentionally omitted and replaced with a single circular hole. The two waveguides flanking the cavity are positioned at a distance from it, defined by two holes. When the analyte is introduced into the sensing region, the resonant wavelength of the device shifts towards the higher wavelength region. This shift results in significantly enhanced sensitivity levels. The proposed biosensor's performance is evaluated using the Plane Wave Expansion (PWE) method and the Finite-Difference Time-Domain (FDTD) tool within the RSoft Photonic Suite CAD [5].

To support our discussion, we will rely on key scientific references that have shaped the evolution of this cutting-edge technology. Relevant research works include the studies by Gowda et al. (2023) [20], which demonstrated the effectiveness of a photonic crystal sensor for detecting bacteria in drinking water, and the research by Vahid Fallahi et al. (2023) [21] on optimizing photonic crystals for increased sensitivity. These references testify to the diversity and vitality of research in this rapidly expanding field.

2. PROPOSED DESIGN

Numerical techniques were employed for the design and simulation of the proposed optical sensor. To determine the photonic band gap (PBG) of the initial photonic crystal (PC) structure, the plane wave expansion (PWE) method was utilized. This approach relies on frequency analysis within periodic environments [22]. The rationale behind selecting this method lies in its ability to directly create a PBG without the need for converting between the time domain and frequency domain. Conversely, the finite-difference time-domain (FDTD) method was employed to analyze the simulated structure. In this method, electromagnetic field equations are discretized using the Taylor series. An important feature of this technique is its capability for parallel data processing, which significantly reduces computation time [23].

To construct the initial configuration of the PC sensor, we arranged 21×13 silicon rods in a periodic pattern within the XZ plane (radius constant = 0.450 μm). The two-dimensional arrangement of these rods forms a hexagonal lattice with a lattice constant of 0.190 μm. This structure exhibits one photonic band gaps (PBGs) in TM mode. The TM mode encompasses a wavelength range from 1.2427 μm to 1.7659 μm, a range particularly suitable for electronic and telecommunication applications.

This intricate sensor structure, designed within the triangular lattice framework, consists of a hexagonal cavity situated between two waveguides. These waveguides are formed by the removal of two rows of air holes each characterized by a radius $r2$ along the ΓK direction on both sides of the central cavity [24], They are used to couple light in and out of the pho-

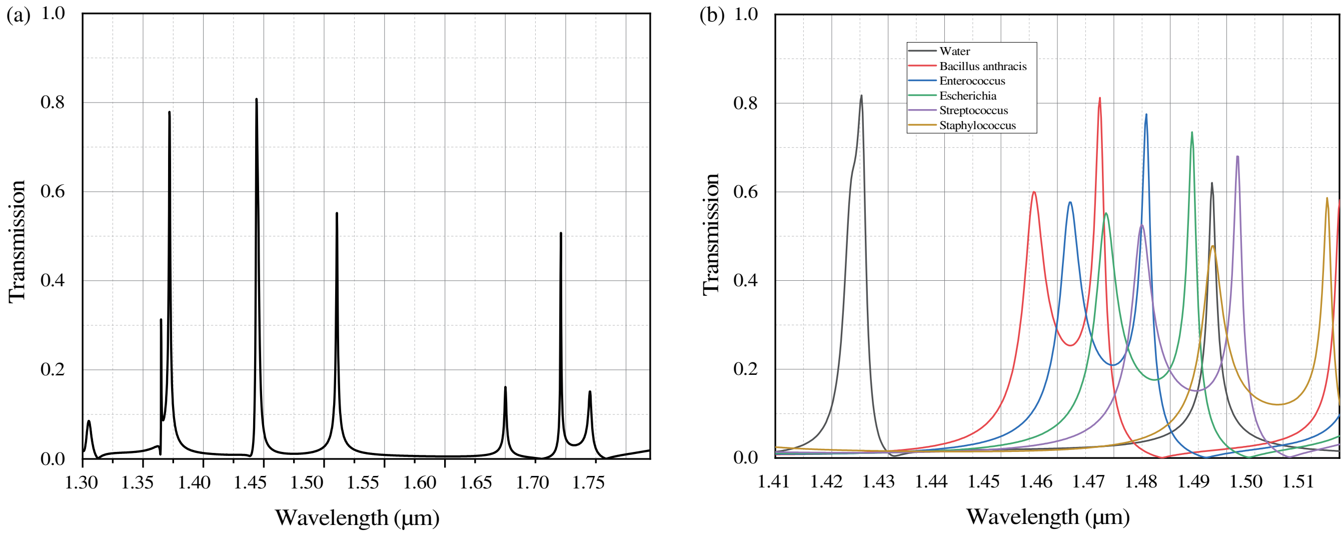

FIGURE 2. (a) Transmission spectra for normal water. (b) Transmission spectrum recorded by the detector for various bacteria.

tonic crystal cavity (CPh). For a comprehensive understanding of the sensor's cross-sectional representation, refer to Figure 1.

During the simulation, a Gaussian light source with a center frequency and width aligned with the photonic band gap was placed on the left side of the sensor system and allowed to propagate through several periods. The transmission spectrum of the system was monitored by observing the output pulse on the opposite side of the sensor [25–30]. The excitation light propagates in the first waveguide and couples to the second through the cavity. This light is then detected at the output of the waveguide. Through the cavity, this type of coupling allows for the extraction of one or several frequencies propagating in the input guide. These frequencies can subsequently be redirected, in a directional manner, towards the second guide also juxtaposed to the cavity.

Figure 1 provides a schematic depiction of the sensor's cross-section. In this representation, the sensor is constructed within a triangular lattice consisting of air holes with a fixed radius of $R = 0.19\,\mu\text{m}$. To create the central cavity, every seventh hole in the middle of the lattice structure was omitted, subsequently replaced with a single circular hole each charachterized by a radius R Surrounded by holes with a radius of $r1$. The two waveguides flanking the cavity are separated from it by two holes each characterized by a radius: $r3$.

3. RESULTS AND DISCUSSION

During our simulations, we observed that our structure displays various resonance modes, each corresponding to a specific frequency at which light waves are greatly amplified when interacting with the crystalline structure of the sensor. Among these modes, we specifically identified and chose the resonance mode around 1.45 μm, see Figure 2(a).

The choice of the specific resonance mode is motivated by the optimal alignment of our sensor with the structural characteristics of the bacteria we aim to detect in drinking water. This particular mode offers maximum sensitivity, meaning that the sensor reacts very precisely to the presence of the targeted bacteria. By focusing our attention on this resonance mode, we ensure to maximize the accuracy of detecting bacterial contaminants in the water sample. In other words, the careful selection of this resonance mode allows for an optimal synergy between the specific structural properties of the targeted bacteria and the sensor's ability to detect them with increased sensitivity.

We can get different transmission spectrums as an output of simulation in this work. The transmission spectrum obtained for the various bacteria present in the test sample is shown in Figure 2(b). We can observe that there is a shift in the wavelength for every bacterial detection.

The sensitivity of a photonic crystal sensor is directly linked to the optimization of its geometric parameters. By adjusting the crystal's geometry, such as hole size, lattice constant, or structure shape, one can influence how light interaction with the sensor. Precise optimization of these parameters allows for tuning the sensor's optical resonance, thereby enhancing its ability to detect small variations in the refractive index of the environment. In other words, by geometrically optimizing the sensor, its sensitivity is maximized, thus improving its performance as a detection device.

To achieve an optimal design, the values of R of the improved structure are adjusted, and the results are presented in Figure 3(a). Consequently, the optimal value for R is chosen to be 1.8 μm. Figures 3(b)–(f) show the magnetic field distributions (H-field) of the resonant modes when R varied from 175 nm to 195 nm, here the refractive index of the holes is 1.38 (which present the appearance of Bacillus anthracis in the water). It can be seen that the magnetic field of peak 1 is mainly distributed in the high refractive index region away from the central hole, so peak 1 is insensitive to the alteration of the refractive index around the surface of the central hole.

The magnetic field of peaks 2, 3, 4, and 5 is concentrated in central hole, so these resonant modes are sensitive to the alteration of the refractive index around the surface of the central hole. But it is clear that the magnetic field of peaks 2 and 3 is precisely distributed on the surface of the central hole, which

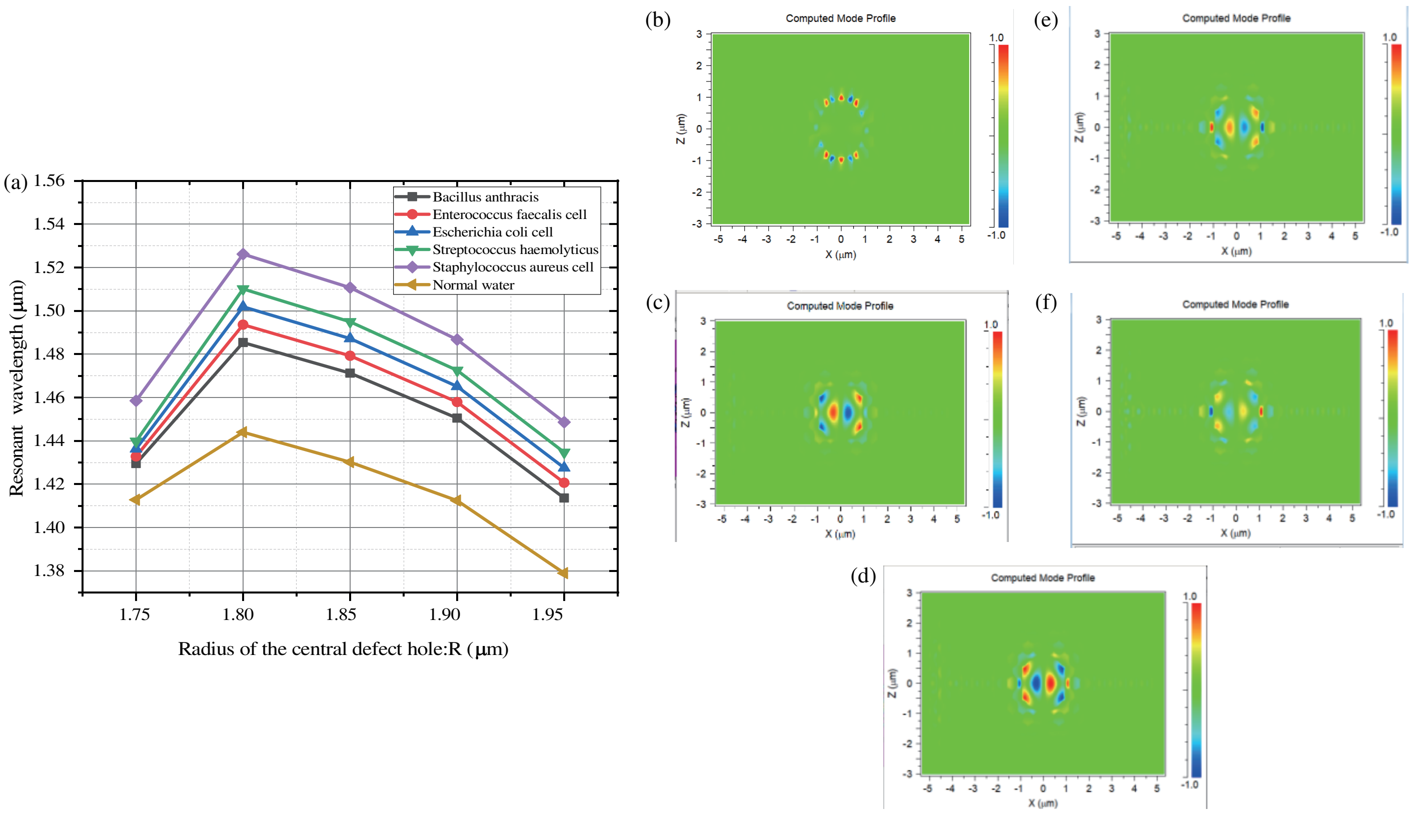

FIGURE 3. a) Values of the alteration of resonant wavelengths when the central hole radius "R" is varied by a 50 nm from 175 nm to 195 nm for different refractive index. (b)–(f) Spatial field distribution of resonant mode for different R. (b) $R = 1.75$ μm, $\lambda_1 = 1.4295$ μm. (c) $R = 1.8$ μm, $\lambda_2 = 1.4854$ μm. (d) $R = 1.85$ μm, $\lambda_3 = 1.47121$ μm. (e) $R = 1.9$ μm, $\lambda_4 = 1.45051$ μm. (f) $R = 1.95$ μm, $\lambda_5 = 1.4136$ μm.

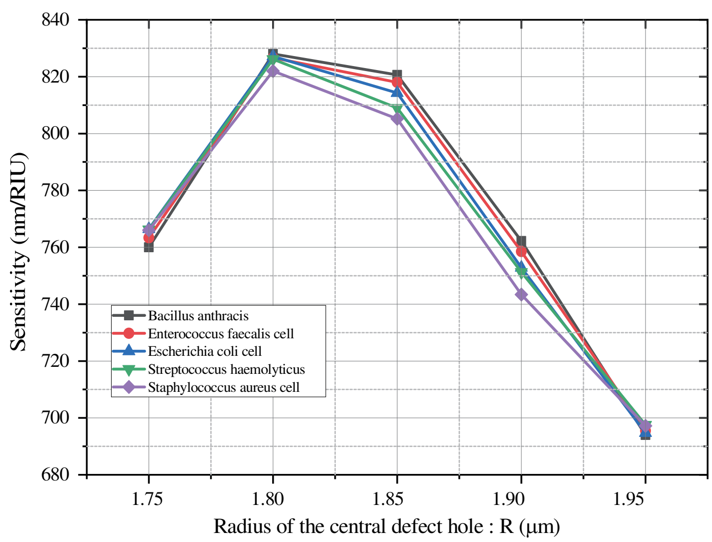

FIGURE 4. The variation of the sensitivity according to the change of the central hole radius R.

is very helpful for enhancing the performance of the drinking water quality monitoring sensor. The magnetic field of peaks 2 and 3 is distributed within the central hole and the area at a surface around the central hole, which means that it would be more sensitive as the presence of the bacteria in the water.

So, when the cavity is in a state of resonance, the distinct peaks emerge within the photonic bandgap (PBG) at the resonance wavelength. At this moment, the electromagnetic field is tightly confined within the cavity, thereby generating heightened sensitivity to changes in the refractive index. This sharp resonance enhances the light-matter interaction, making the cavity highly responsive to variations in the refractive index.

The variation tendencies of the sensitivity according to R change from 175 nm to 195 nm are plotted in Figure 4. Accord-

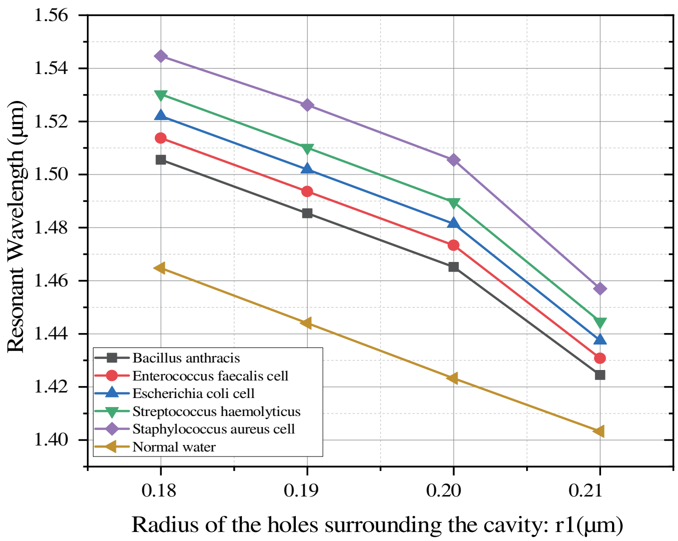

FIGURE 5. The variation of the resonant wavelength with changes in the surrounding hole radius of the cavity: $r1$.

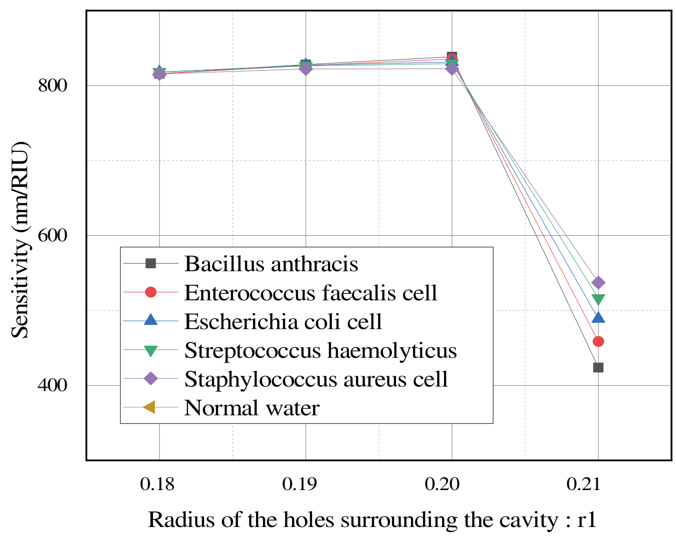

FIGURE 6. The variation of sensitivity with changes in the surrounding hole radius of the cavity: $r1$.

TABLE 1. Transmission spectrum data.

Bacteria Type	Refractive Index	Resonant Wavelength (μm)	Sensitivity (nm/RIU)
Bacillus anthracis	1.38	1.4653	840.8
Enterococcus faecalis cell	1.39	1.4736	839
Escherichia coli cell	1.40	1.48168	834.57
Streptococcus haemolyticus	1.41	1.48984	832.25
Staphylococcus aureus cell	1.43	1.50577	825.1
Normal water	1.33	1.42326	ref

ing to the simulation results, we can note that, by increasing the radius of the central defect hole, the sensitivity gets promoted with the increase of R followed by a slight decrease, and as seen the hole radius of $R = 1.8\,\mu\text{m}$ leads to an optimal design with a sensitivity of 828 nm/RIU.

Figure 5 illustrates how the resonance wavelength varies with the variation of $r1$. By observing this figure, it can be noted that the resonance wavelength gradually decreases as the value of $r1$ increases, indicating a reduction in the detection area. This gradual decrease is explained by the progressive reduction of the interaction between optical modes and the analyte.

While the optimal value of $r1$ is selected based on Figure 6, which depicts the sensitivity variation with $r1$, there is an observed increase in sensitivity with the increment of $r1$ until it reaches the value of 0.20 μm, followed by a notable decrease.

Similarly, regarding the variation of resonance wavelength and sensitivity with respect to $r2$, as illustrated in Figures 7 and 8, the optimal value for $r2$ is 0.18 μm with $r3 = 0.19\,\mu\text{m}$.

Upon introducing diverse bacterial components into the cavity, alterations in cavity refractive index lead to corresponding changes in transmission characteristics. As previously emphasized, the paramount performance metric for this sensor is its sensitivity. It is the ratio of resonant wavelength changes to the RI change of the test sample and is denoted as

$$S = \Delta\lambda/\Delta n \tag{1}$$

where $\Delta\lambda$ is the resonant wavelength shift, and Δn is the change in RI of the test sample.

These critical parameters for the engineered structure are meticulously detailed in Table 1.

Table 1 offers a comprehensive summary of the sensor's performance when it is exposed to various bacterial species in the test sample. An examination of the table data reveals that the proposed resonator structure achieves its peak sensitivity values, measuring 840.8 μm/RIU and 839 μm/RIU, correspondingly, in response to Bacillus anthracis and Enterococcus faecalis cell.

Table 2 clearly demonstrates that the proposed structure exhibits superior sensitivity compared to other existing sensors. Based on the results obtained, it can be confidently asserted that the proposed structure is highly effective as an optical sensor for the detection of five distinct bacterial types in the sample.

4. FUTURE PERSPECTIVES

The technology of photonic crystal sensors represents an innovative approach to assess the purity of drinking water, playing a crucial role in ensuring the quality of our water supply. This

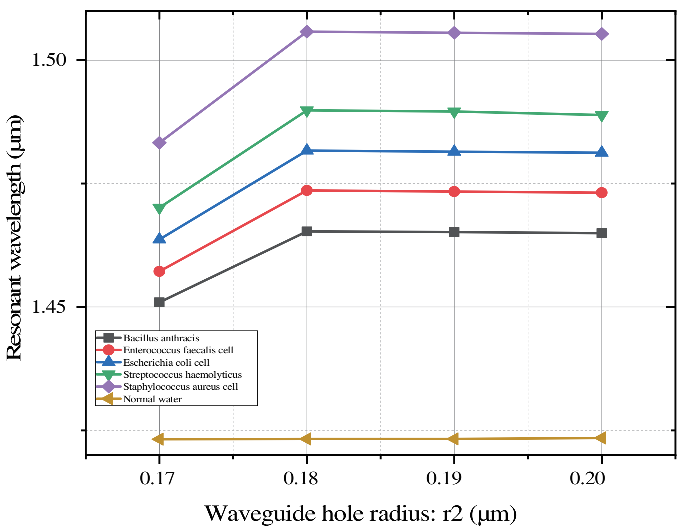

FIGURE 7. The variation of resonant wavelength with changes in waveguide hole radius: $r2$.

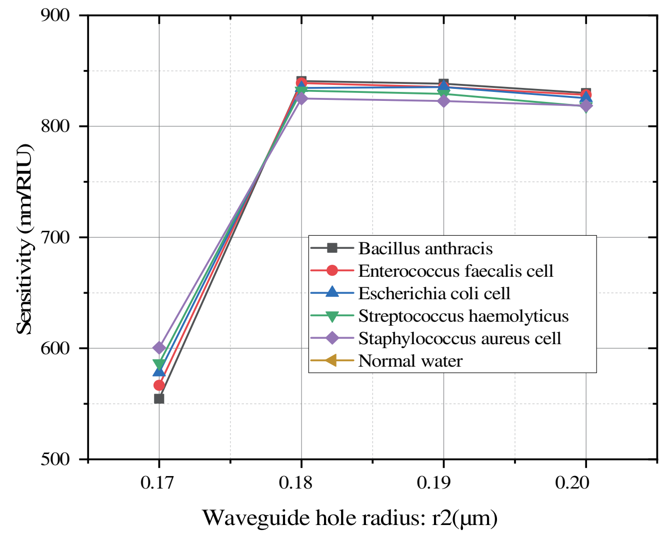

FIGURE 8. The variation of the sensitivity with changes in waveguide hole radius: $r2$.

TABLE 2. A comparative analysis of the sensitivity between the proposed design and the findings documented in the literature.

References	Sensitivity	Published year
[25]	300	2019
[22]	435	2015
[31]	610	2023
[21]	756	2023
[20]	201.5	2023
Current work	834.344	

study explores potential extensions of this technology, examines its possible applications, and identifies areas requiring further investigation.

A major evolution of our sensor technology would involve expanding the range of detectable contaminants. Currently focused on water purity, the technology could be adjusted to monitor specific components such as heavy metals, organic chemicals, or other emerging contaminants, thereby enhancing its utility in safeguarding the overall quality of water.

Our structure could find applications in various aspects of water monitoring. It could be integrated into distribution systems for real-time contamination detection, thereby improving the responsiveness of water management authorities. Furthermore, it could be employed in portable devices, enabling individuals to verify water quality at the source.

5. CONCLUSION

This study focuses on the design and simulation of a biosensor based on photonic crystals to detect five different types of bacteria in drinking water: Staphylococcus aureus, Streptococcus hemolytic, Escherichia coli, Enterococcus faecalis, and Bacillus anthracis. The Rsoft software is used to design and analyze the proposed sensor structure. Measurements and analysis of transmission spectra are conducted for various water samples containing different pathogens, varying the values of the refractive index. This enables the precise determination of water purity. The presence of bacteria can be detected and identified by observing the shift in wavelength of the transmission spectrum as well as the refractive index value of the analyte. This structure, easy to design, exhibits increased sensitivity ($S = 834.344$ μm/RIU), and superior accuracy in detecting pathogens in water. Therefore, it is easy to detect the presence of bacteria in the sample by directly observing the shifts in the transmission spectrum.

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