DESIGN AND ANALYSIS OF A PHOTONIC CRYSTAL-BASED BIOSENSOR INTEGRATED WITH MACHINE LEARNING FOR HUMAN PAPILLOMAVIRUS DETECTION IN URINE

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Introduction:

Cervical cancer is the fourth most common cancer in women globally. It starts in the cells of the cervix and is caused by infection with the human papillomavirus (HPV). The Screening of this cancer involves Pap smear, DNA detection in cervical cells, etc. All screening methods are invasive and require medical expertise, thus creating a barrier to widespread screening programs. Hence, urinary HPV testing, being a non-invasive method can offer logistical advantages, high acceptability, and reducing barriers related to screening coverage.

The photonic biomolecular biosensor will be designed to capture the HPV cancer-specific analytes. Photonic crystal-based devices have become essential building blocks for the photonics community in sensing, communication systems, and quantum applications. The literature survey revealed that no studies have used this technique hitherto to detect HPV DNA in urine. This study intends to design a biosensor-based urinary testing for HPV virus detection.

Objectives:

1. To *design and simulate* a Photonic crystal-based biosensor structure that can detect the Human Papillomavirus (HPV) in urine.
2. To *investigate* the parameters like sensitivity, quality factor (Q-factor), figure of merit (FOM) and limit of detection (LOD) of the biosensors for HPV virus detection and repeating the design to improve those design parameters by changing different design constraints.
3. To *optimize* the design and parameters of the biosensors to achieve higher accuracy and reliability.
4. To *compare* the performance of the developed photonic crystal-based biosensors with existing biosensor technologies for the detection of HPV virus.
5. To *verify* the simulation results and enhance prediction accuracy by applying machine learning algorithms, ensuring robust analysis and validation of the biosensor's performance.

Overall, the project's objectives are to design, simulate, optimize, and verify photonic crystal-based biosensors that can detect HPV virus in urine samples with high sensitivity, quality factor, and limit of detection. The project aims to contribute to the field of biosensors and provide a potential tool for healthcare professionals to monitor cancer and overall health.

Methodology:

The proposed work involves the design of a device intended to act as a detection system for the HPV virus in urine. A Gaussian light source will pass through the Photonic crystal through the input port. The propagation of electromagnetic waves takes place within the sensor device. Depending upon the Refractive index values of the HPV virus, the propagation of light will vary and hence its optical properties will change. The change in the Refractive index causes wavelength shift. A Photonic crystal-based biosensor works on the principle that a change in the concentration levels of HPV virus in urine changes RI, which changes the output response which in turn causes the wavelength to shift. Then the output waveforms are compared with their pure ones. Then the wavelength shift, Quality factor, limit of detection, figure of merit, and sensitivity are observed. Further, the classification of cells and probability of cells with HPV cancer can be detected and verified using a logistic regression algorithm (LRA).

The steps followed to simulate this work are as follows,

- A comprehensive review of the existing literature on photonic crystal-based biosensors will be conducted to identify the research gaps, design concepts, and optimization parameters.
- Design a photonic crystal resonator-based biosensor with the dimensions required for the detection of HPV virus using Ansys Lumericals/ Comsol/ MEEP software.
- Refractive index (RI) values of the HPV virus are collected.
- The sample RI values are given to the holes in the structure representing the urine sample on the sensor holes
- Analysis of the electromagnetic field propagation of the sensing devices is carried out by the Finite Difference Time Domain (FDTD) method to obtain the optimized design structure.
- Optimize the device for high sensitivity, Q-factor, and intensity using the FDTD method.
- Analyze the biosensor by applying bio properties of cervical cancer in urine using the FDTD method.
- With the change in RI, the resonant wavelength shifts. These shifts are observed, graphs are plotted and readings are tabulated for different parameter values.
- Finally the simulation results are verified by applying a machine learning algorithm like linear regression algorithm that validates the biosensor's performance.

Result and Conclusions:

In the photonic crystal, a resonator is a structure that traps and concentrates electromagnetic energy at a specific frequency. Resonators are typically made of a defect or perturbation in the periodic structure of the photonic crystal. This defect creates a localized mode of electromagnetic energy that is confined within the resonator. The resonator can be designed to have a frequency that matches a specific wavelength of light, and can therefore be used to selectively enhance or filter light at that frequency.

A hexagonal ring resonator will be designed for photonic devices that can be used as sensors. It consists of waveguides, typically made of a high refractive index material such as silicon, which is connected to straight waveguides. In a hexagonal ring resonator, Light is coupled into the hexagonal resonator through the straight waveguides, and it circulates the hexagonal ring before being coupled out through the output waveguide.

From the literature survey, a hexagonal ring resonator structure is used for the proposed application. Figure 1, shows the structure considered for Hexagonal Resonator Structure for a photonic crystal based biosensor.

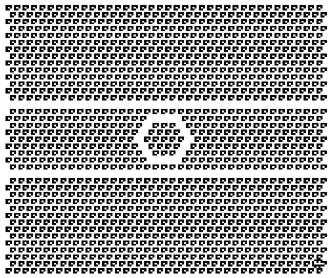

Figure 1: Proposed sensor structure

Table 1 shows the design parameters used for the proposed hexagonal biosensor structure.

Table 1. Design Parameters

Sl. No	Parameter	Values
1	Configuration	Holes In Slab
2	Structure of the Lattice	Hexagonal
3	Silicon Thickness	220nm
4	L1 Hole Radius	0.18 µm
5	L2 Hole Radius	0.1 µm
6	L3 Hole Radius	0.03 µm
7	Remaining Hole Radius	0.123µm

8	Lattice constant	0.35µm
10	Refractive index (RI) value of Si	3.46

By doing analysis, we have finalised the design parameters and then designed the hexagonal ring resonator structure accordingly as shown in Figure 2 using Ansys Lumericals Software. Next we have to optimize the structure for maximum performance parameters and then validate the simulation by using machine learning algorithm.

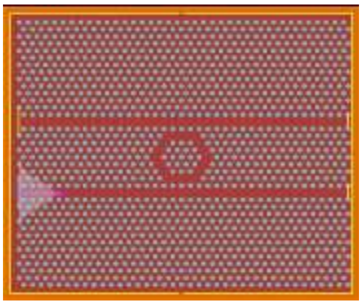

Figure 2: Designed hexagonal ring resonator structure

Q-factor is calculated using eq. 1, sensitivity is calculated using eq. 2, and FOM is calculated using eq. 3 and LOD is calculated using eq. 4.

$$Q = \frac{\text{Resonant wavelength}}{\text{FWHM(3−db BW of the spectral range)}} \quad (1)$$

$$\text{Sensitivity (S)} = \frac{\text{Change in wavelength}}{\text{Change in the RI value}} \quad (2)$$

$$\text{FOM} = \frac{S}{\text{FWHM}} \quad (3)$$

$$\text{LOD} = \delta n = \frac{FWHM}{1.5\,(S)SNR^{0.25}} \quad (4)$$

In conclusion, using defect engineering, a hexagonal ring resonator structure is created. A Photonic crystal-based biosensor works on the principle that a change in the concentration levels of HPV virus in urine changes the output response which in turn causes the wavelength to shift. A Finite Difference Time Domain (FDTD) based tool called Ansys Lumericals is used for the simulation. Performance parameters like

Quality factor (Q-factor), Sensitivity, Full width at half maximum (FWHM), Figure of Merit (FOM), and Limit of Detection (LOD) are calculated. Then the simulation results are verified by applying a machine learning algorithm like a linear regression algorithm ensuring robust analysis and validation of the biosensor's performance.

The novelty of the work is to detect HPV virus using a PhC structure design. Furthermore, combining machine learning with photonics is a novelty. Proper designing and analysis of these sensors show many crucial benefits like remarkable sensitivity, Q-factor, good accuracy and inherent miniaturization which may lead to the possible patentability and provide proper simulation evidence for guiding the fabrication process and developing the final device.

Future Scope:

The future scope of this project includes:

1. There is growing interest in identifying optical biosensors to detect human papillomavirus from urine samples, which might address the detection of HPV virus infections.
2. A statistical analysis of the collected data reveals that limited studies have been reported on photonic crystal-based biosensors for HPV detection. This work contributes to the existing knowledge by providing simulation evidence, which is crucial for guiding the fabrication process and developing the final device.
3. Experimental Fabrication and Testing.

Project Outcome & Industry Relevance (10-15 lines):

1. There is growing interest in identifying optical biosensors to detect human papillomavirus from urine samples, which might address the detection of HPV virus infections.
2. Publication in a Scopus-indexed IEEE conferences or peer-reviewed journals
3. A potential patent application for the developed biosensor design.

Industry Relevance:

1. This project contributes to the field of optical biosensing by offering a compact, non-invasive, and highly sensitive detection method. The design's miniaturization and accuracy make it suitable for future development into portable diagnostic devices. In real-world settings, such biosensors could be integrated into point-of-care diagnostic systems in hospitals, clinics, or even home-use kits.
2. Industries involved in biomedical diagnostics, healthcare technologies, and lab-on-chip systems could greatly benefit from this sensor. Moreover, the methodology and simulation results offer a foundation for further development, prototyping, and eventual commercialization, showing promise for patentability and future research collaborations.

Working Model vs. Simulation/Study:

This project is currently a simulation-based study and does not involve the development of a physical working model at this stage. All analyses, performance evaluations, and validations were carried out using Finite Difference Time Domain (FDTD) simulations through Ansys Lumericals. The results provide a strong theoretical foundation, which can guide future experimental fabrication and testing.