

ANALYSIS OF FLUORIDE DETECTION IN WATER USING PHOTONICS BASED BIOSENSORS

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Abstract— Optical biosensors are highly sensitive devices for detection and analysis of bio-analytes that combines biological components with a physicochemical detector. Biosensors have vast applications in biomedical research, environmental monitoring, healthcare, and pharmaceuticals. In this paper we have demonstrated a 2-dimensional photonic crystal based biosensor with line defect which can detect different fluorides in water. Simulation and analysis has been done for calcium fluoride, cesium fluoride, potassium fluoride, lithium fluoride and strontium fluoride and peak has been observed. By detecting these fluorides various diseases that are caused by fluorides can be detected easily. One such major detection is to detect dental fluorosis caused by the fluorides present in water. Finite Difference Time Domain (FDTD) method has been used for the analysis. MEEP (MIT Electromagnetic Equation Propagation) simulation tool have been used for modeling and designing of photonic crystal. It has been observed from the band structure that for little change in refractive index (RI) there will be a moderate shift in the frequency and hence it acts as a sensor. This indicates that it is highly sensitive for the change in refractive index. The quality factor of the design is found to be 134897.

I. INTRODUCTION

Dental fluorosis is a alteration in the advent of the tooth's enamel. These variations can vary from hardly perceptible white spots in mild forms to staining and pitting in the more severe forms. Dental fluorosis only occurs when younger children devour too much fluoride, from any source, over long periods when teeth are evolving under the gums. The advantageous effects of fluoride on dental caries are due predominantly to the topical effect of fluoride after the teeth have vented in the oral cavity. In dissimilarity, disadvantageous effects are due to systemic absorption during tooth development subsequent in dental fluorosis.[1]In India, fluorosis was recognized in 1937 in Nellore of Andhra Pradesh by Shortt et al.[2] Geological crust of India, especially South India, has fluoride rich bearing minerals which can taint underground aquifers.[3] Nearly 73% of Tamil Nadu is hard rock crust.[4] In Tamil Nadu, Madurai is a known endemic fluorosis area and has fluoride level in drinking water of about 1.5 - 5.0 ppm.[5].

The earliest manifestation of dental fluorosis is an increase in enamel porosity along the striae of Retzius.[6]. Clinically, the porosity in the subsurface of enamel reflects as opacity of the enamel. With an increased exposure to fluoride during tooth formation, the enamel exhibits an increased porosity in the tooth surface along the entire tooth surface. Very severely hypo mineralized enamel will be very fragile and hence as soon as they erupt into oral cavity they undergo surface damage as a result of mastication, attrition and abrasion. The definite evidence that fluoride can induce dental fluorosis by affecting the enamel maturation was given by Richards et al.[7] Thylstrup and Fejerskov proposed a way of recording dental fluorosis (TF index) based on the histopathological features.[8] Human and animal studies have shown that the enamel hypomineralization in fluorotic teeth are due to aberrant effects of fluoride on the rates at which enamel matrix protein breakdown or rates at which the byproducts of enamel matrix degradation are withdrawn, resulting in retardation of crystal growth in enamel maturation stage.[9]Fluorosis is a major health problem in India with over 65 million people at risk and 6 million children seriously affected.[10]

II. THEORY

Photonic crystals arise from the cooperation of periodic scatters - thus, they are called crystals because of their periodicity & photonic because they act on light. They can occur when the period is on the order of the wavelength of light. Photonic crystals are defined as regular arrays of materials with different refractive indices & are attractive optical materials for controlling & manipulating the propagation of electromagnetic waves in the same way as the periodic potential in a semiconductor crystal affects the electron motion by defining allowed & forbidden electronic energy bands. The concept behind the photonic sensing technology is that each material has distinct permittivity 'ε' that is greater than air, as a result the propagation of electromagnetic waves that pass through them is altered, in response to change in refractive index.

The photonic band gap structure for the photonic crystal defines its optical properties and is obtained by plotting the resonant frequency against the 'k' wave vector. The photonic band gap acts as 'optical insulator' [11]. The photonic band gap property can be explored for sensing applications. The photonic band gap property can be altered by creating defects in the photonic crystal [11][12]. Defects can be created either by changing the dimension or dielectric constants of one or more group of elements or removal from the structure and act as optical cavities. Defects control the flow of light inside the photonic crystal. Defects can be point defect or line defect. Light can be localized at a point in photonic crystal with the use of point defect, while in line defect the inhomogeneity is extended to create waveguide in the photonic crystal [13][14].

The light is passed through one end of the phonic crystal & the transmission spectrum is observed at the other end. The transmission spectrum observed is unique for the specific fluoride. The photonic integrated circuits (PICs) consist of light sources, sensors & detectors which are integrated on one single chip. Hence, the designed sensor can be fabricated as a lab-on-chip sensor to detect different hazardous fluorides in water.

Different toxic fluorides are used in background of the crystal, as the refractive index varies for different fluorides the refractive index profile changes. Hence the intensity levels of the transmission spectrum changes, thus one can measure peak wavelength of various fluorides.

III. ALGORITHM

The Finite difference Time Domain (FDTD) method is implemented using the simulation tool MEEP. The Finite Difference Time Domain method solves the time domain Maxwell's equation. The method divides the field in time and space and solves for electric and magnetic fields. MEEP is a simulation tool developed by MIT for design, model and stimulate various photonic crystal structures. It is a time domain tool and implements the FDTD method. The transmission and the reflection spectrum are obtained using the MEEP tool. MEEP solves the Poynting vector (Equation 1) and computed the fluxes.

$$P(\omega) = Re \hat{n} \cdot \int E_{\omega}(x)^* \times H_{\omega}(x) d^2x \dots\dots\dots(1)$$

With FDTD approach sampling of continuous electromagnetic field in a finite volume of space takes place. Electromagnetic field is sampled at discrete points in a space lattice and at discrete points in time and different field components can be obtained at different grid locations [13][16]. This discretization of equations with second-order accuracy is known as Yee lattice. MEEP tool implements the finite difference time domain method [14][15].

The propagation of light in photonic crystal is explained by the master equation (Equation 1). The master equation is

obtained by solving Maxwell's electromagnetic equations [11].

$$\nabla \times \nabla \left(\frac{1}{\epsilon} \nabla \times \vec{H} \right) = \left(\frac{\omega}{c} \right)^2 \times \vec{H} \dots\dots\dots(2)$$

In the above Equation (1), 'ε' is permittivity (dielectric function = n² where 'n' is the RI), 'ω' is frequency. The above Equation (1) tells that the frequency 'ω' is inversely proportional to the dielectric function 'ε'.

To find the value of P(ω), MEEP computes the integral P(t) of the Poynting vector at each time, and then Fourier-transform the value obtained. The flux at the specified regions and the frequencies that we want to compute can be computed by MEEP [14].

IV. SENSOR DESIGN

We have proposed a photonic crystal based waveguide structure with rods in air configuration for sensing salmonella typhi. The design of the sensor consists of the two dimensional square lattice waveguide photonic crystal structure in rods (silicon) in air configuration. A straight waveguide is carved out making a simple waveguide [16] structure. The analyte which turns out to be water in this case is absorbed over the surface of the photonic crystal. When the light passes through the photonic crystal the interaction of light and the sample will take place. The light is passed through one end of the phonic crystal & the transmission spectrum is observed at the other end. The propagation of light in the photonic crystal will vary with respect to the different dielectric constants of the sample constituents. Design of the photonic crystal ring resonator device is shown in "Fig. 1" given below:

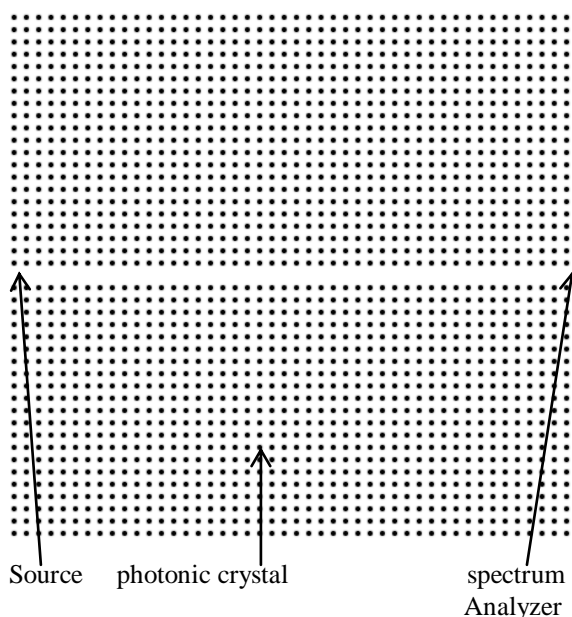


Fig. 1: Design of the photonic crystal based sensor

Designing and simulation is done with the help of MEEP tool. Design Specifications are:

- Square lattice structure with rods in air configuration
- Lattice constant 'a'=0.1 μm
- Radius of rods 'r'=0.25 μm
- Dielectric constant of silicon slab = 11.56
- Dielectric constant of background of the photonic crystal is changed with respect to sample taken
- Gaussian Pulse with center frequency at 0.351 and width of the pulse is 0.25 used as light source
- Wavelength of light taken into consideration is 1550 nm.

V.RESULTS

The transmission spectrum plot for wavelength spectrum is illustrated in the Fig 2. The x-axis indicates wavelength and the y-axis indicates transmission flux for the corresponding wavelength. It can be observed that as the change in the refractive index is slight; the change in the transmission spectrum is visibly distinct, proving the sensor to be very sensitive to sense salmonella typhi in aqueous medium from Fig. 2. The same was worked with respect to frequency in transmission and reflection spectrum. The reflection spectrum with respect to frequency is as shown in fig. 3. To explain the concept of signatures, the zoomed version of transmission spectrum and reflection with respect to wavelength and frequency is as shown in fig. 4 and fig. 5 respectively. From the graphs, it can be observed that as the change in the refractive index is slight; the change in the transmission spectrum is visibly distinct, proving the sensor to be very sensitive to sense the hazardous fluoride.

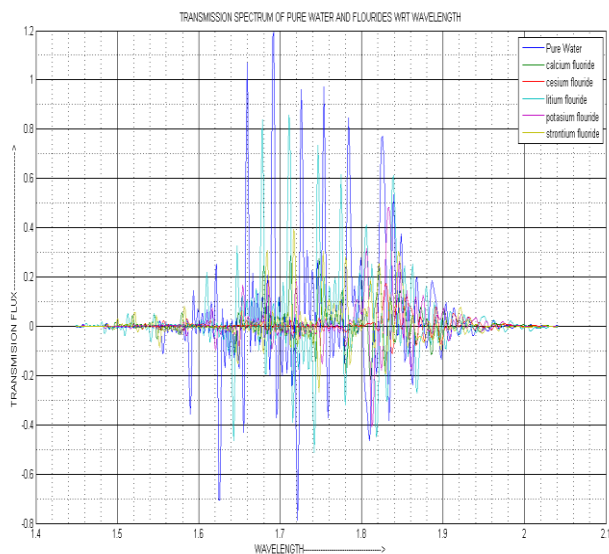


Fig. 2: Transmission spectrum of frequency shift

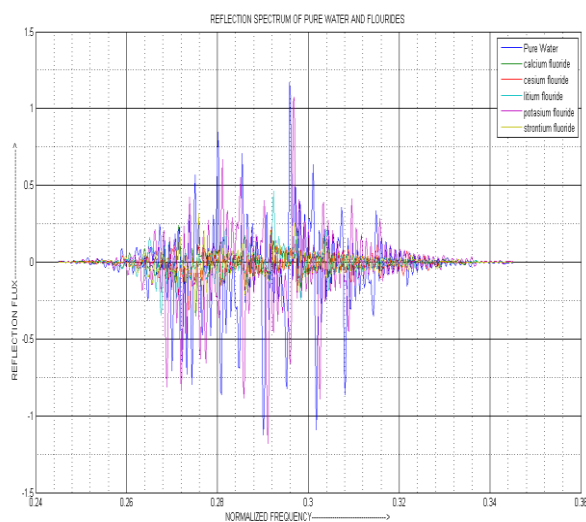


Fig. 3: Reflection spectrum of frequency shift

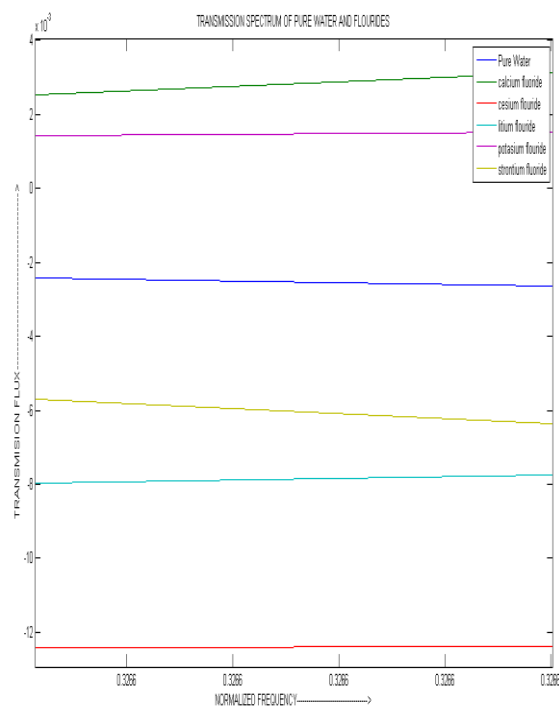


Fig. 4: Zoomed version of transmission spectrum of frequency shift

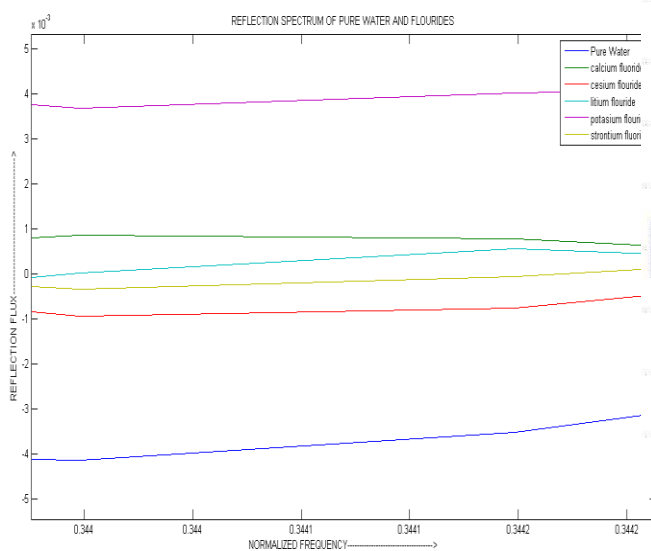


Fig. 5: Zoomed version reflection spectrum of frequency shift

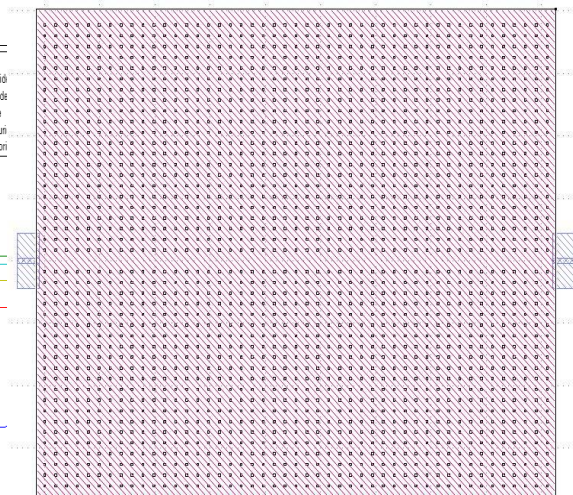


Fig. 7: GDSII file from K-layout

The designed sensor is converted into GDSII file using IPKISS software using python tool and it is viewed in GDSII viewer (OWLVISION) and it is shown in Fig 6. Then it can be easily translated into ASCII format which will be used for fabrication. The GDSII file as shown in figure 4 was then verified with respect to its rulings with the help of K-layout tool and it is shown in Fig 7.

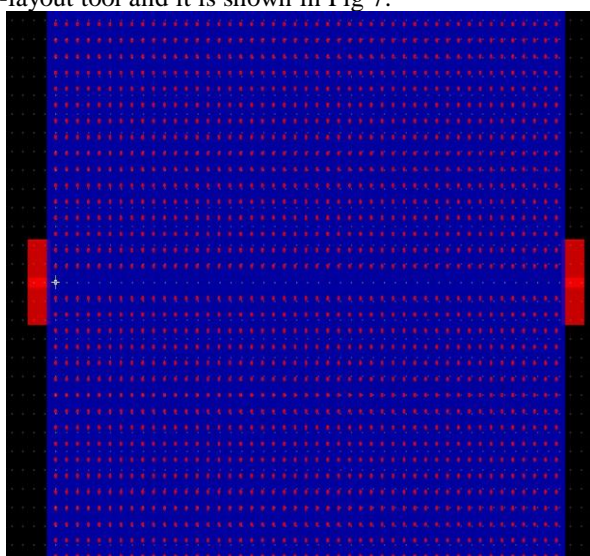


Fig. 6: GDSII file from OWLVISION (GDS viewer tool)

Table 1: shifts in frequency and wavelength spectrum

| | Frequency spectrum (normalized) | | Wavelength spectrum(um) | |
|-------------------------------|---------------------------------|---------------|-------------------------|--------------|
| | trans mission | refl ection | trans mission | reflect ion |
| water without fluoride | 0.2955 | 0.2959 | 1.692 | 1.69 |
| calcium fluoride | 0.2919 | 0.2715 | 1.748 | 1.681 |
| cesium fluoride | 0.2733 | 0.2917 | 1.83 | 1.713 |
| lithium fluoride | 0.2923 | 0.2923 | 1.711 | 1.711 |
| potassium fluoride | 0.2729 | 0.2969 | 1.832 | 1.684 |
| strontium fluoride | 0.2913 | 0.2759 | 1.718 | 1.813 |

The above results define substantial shifts which can thus help in determining the fluorides in water.

VI. CONCLUSION

The sensor design consists of a two dimensional square lattice line defect photonic crystal structure. It is simulated and analyzed for detecting toxic fluorides like calcium fluoride, cesium fluoride, potassium fluoride, lithium fluoride and strontium fluoride present in water that causes dental fluorosis. Visibly distinct shift in both wavelength and frequency are observed, proving the sensor to be sensitive to even a smallest change in the input fluoride. The quality factor was supposedly calculated to be 134897. The line defect structure provides better sensitivity as compared to other photonic crystal design or other optical fiber sensor design.

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