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Detection of Fluoride Contaminated Water in Dental Applications

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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. Groundwater is the major source of drinking water for residents of urban or rural areas. Fluoride content in drinkable groundwater directly affects the quality of drinking water. 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**.

Index Terms— **Globalization, mainframes, CICS, DB2, COBOL**

I. INTRODUCTION

Dental fluorosis is a alteration in the advent of the tooth's enamel. These variations can vary from hardlyperceptible 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.]

II. THEORY

Optics can be defined as the branch of physical science which deals with the generation and propagation of light and its interaction with matter. 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 '€' 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

MEEP is Maxwell's Electromagnetic Equation Propagation simulation tool. MEEP has been programmed by D.Roundy, M.Ibanescu, P.Bermel&S.G.Johson at the Massachusetts Institute of Technology (MIT). MEEP is a time domain tool. MEEP tool implements the finite difference time domain method. Simulation in 1D,2D, 3D & spectral coordinates can be done by using MEEP. The application of FDTD method is computation of transmission spectrum. MEEP is simulation package for the computation of transmission/reflection spectra, field patterns, resonant modes & frequencies in dielectric structures. The transmitted flux can be computed at each frequency ω. For fields at a given frequency ω, this is the integral of the Poynting vector, over a plane on the far side of the photonic crystal structure:

………………….(1)

MEEP computes the integral P(t) of the Poynting vector at each time, and then Fourier-transform this to find P(ω). MEEP computes the flux at the specified regions, and the frequencies that you want to compute. MEEP uses "dimensionless" units, where all εo, μo and 'c' constants are unity. The transmitted amplitude values for corresponding frequency can be extracted from the MEEP output file using the UNIX command 'Grep'. These transmitted amplitude values are plotted against frequency values using MATLAB to obtain the transmission spectrum.

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].

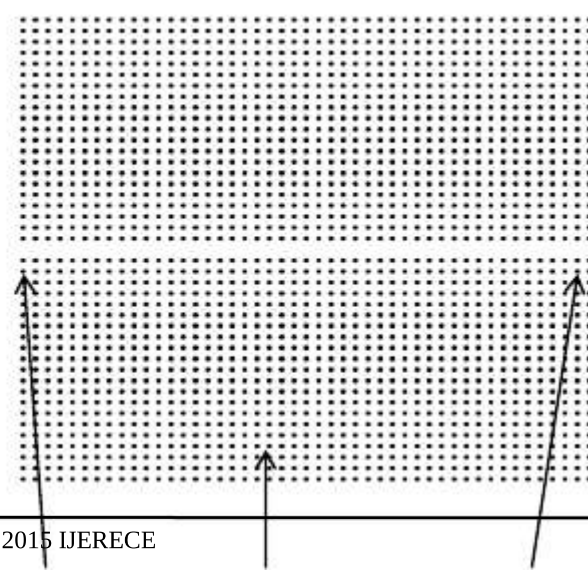
$$\nabla \times \nabla\left(\frac{1}{\in}\nabla \times H\right) = \left(\frac{\omega}{c}\right)^2 \times H \text{ ………………….(2)}$$

In the above Equation (1), '∈ ' is permittivity (dielectric function = n^2 where 'n' is the RI), 'ω' is frequency. The above Equation (1) tells that the frequency 'ω' is inversely proportional to the dielectric function '∈ '.

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

The design of the sensor consists of the two dimensional square lattice waveguide photonic crystal structure in rods 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:



Source photonic crystal spectrum Analyzer

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 um
- Radius of rods 'r'=0.25 um
- 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 for frequency spectrum is illustrated in the Fig 4. The x-axis indicates frequency and the y-axis indicates transmission flux for the corresponding frequency. 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. 4. The same was worked with respect to wavelength in transmission and reflection spectrum. The reflection spectrum with respect to frequency is as shown in fig. 5. To explain the concept of signatures, the zoomed version of transmission spectrum and reflection with respect to frequency is as shown in fig. 6 and fig. 7 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. The zoomed version of transmission spectrum and reflection with respect to wavelength is as shown in fig. 10 and fig. 11 respectively.

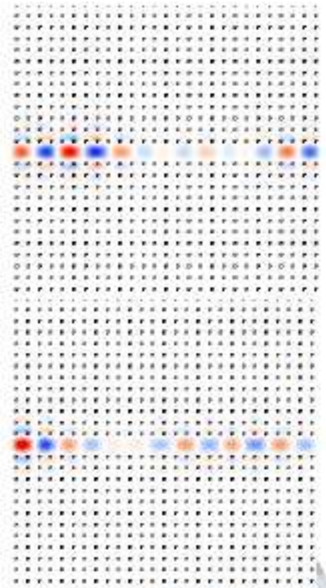


Fig. 2: Simulated images for water.

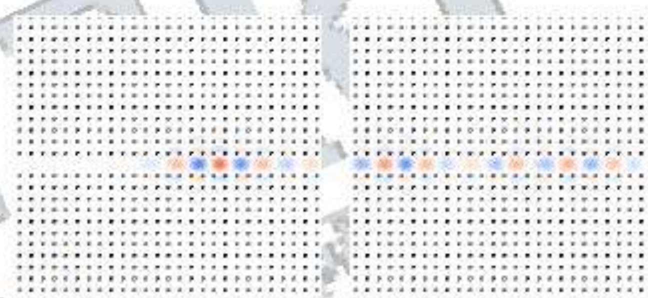


Fig. 3: Simulated images for Fluoride water.

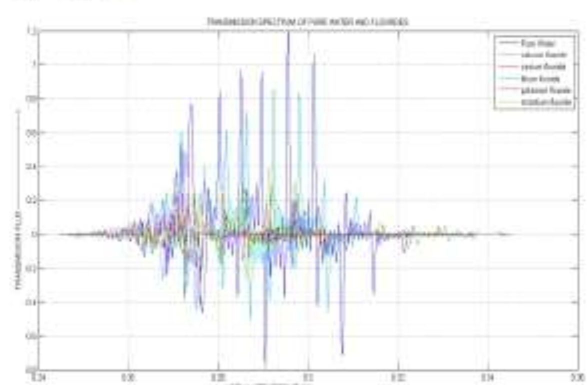


Fig. 4: Transmission spectrum with respect to frequency

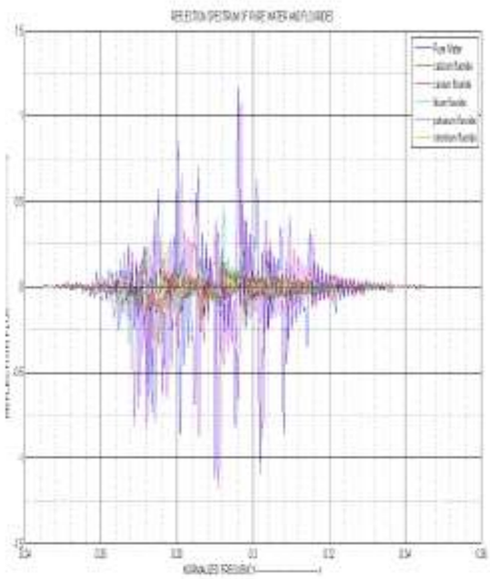


Fig. 5: Reflection spectrum with respect to frequency

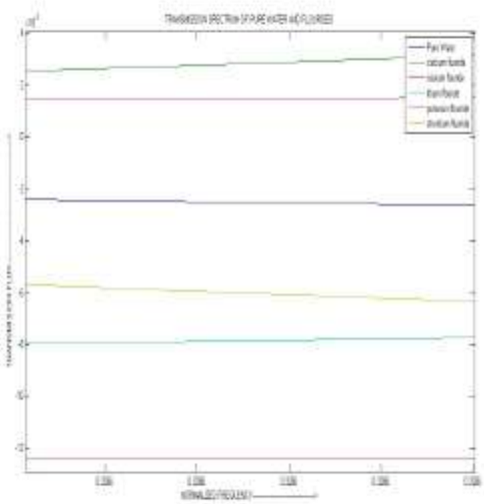


Fig. 6: Zoomed version of transmission spectrum of frequency shift

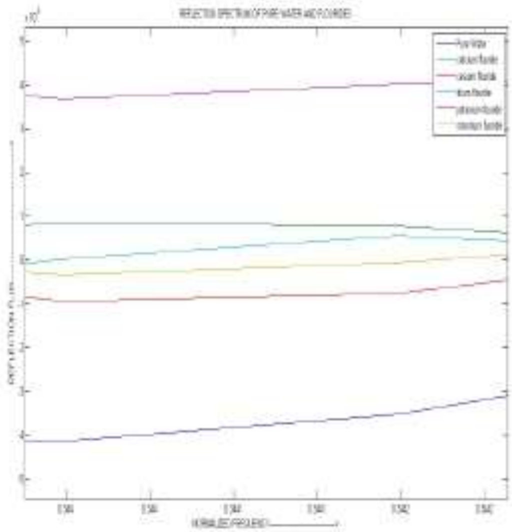


Fig. 7: Zoomed version of reflection spectrum of frequency shift

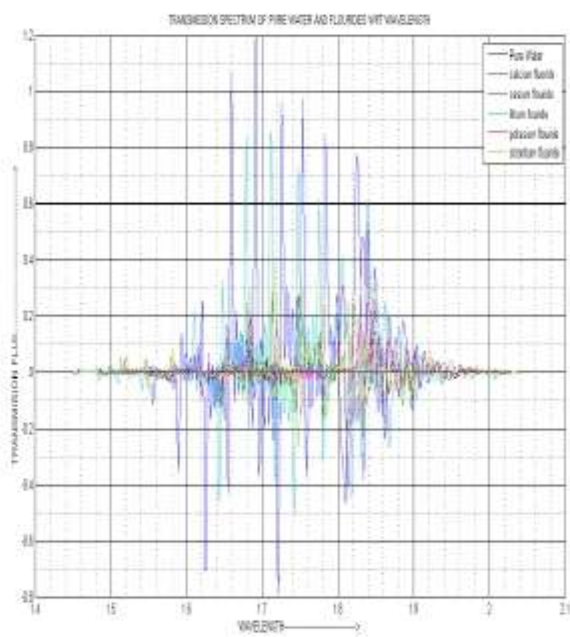


Fig. 8: Transmission spectrum with respect to wavelength

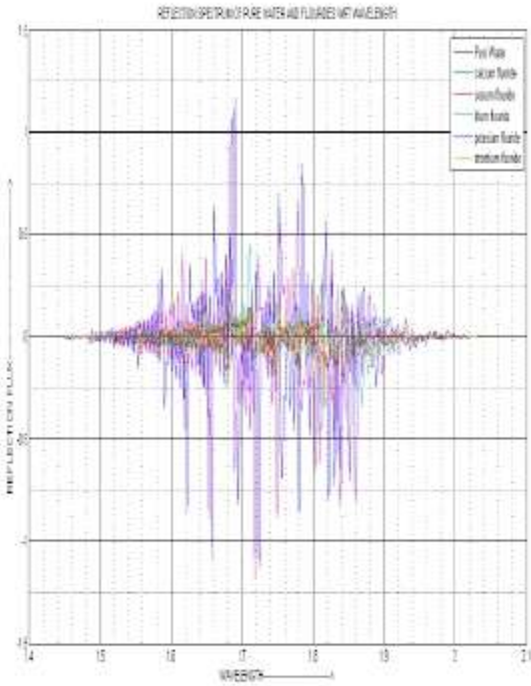


Fig. 9: Reflection spectrum with respect to wavelength

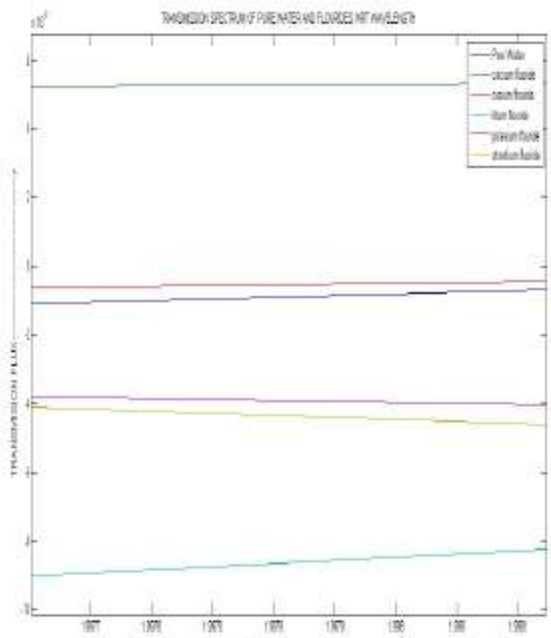


Fig. 10: Zoomed version transmission spectrum of wavelength shift

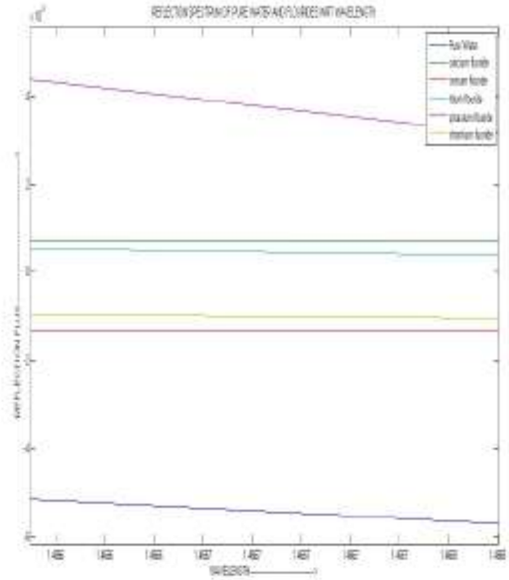


Fig. 11: Zoomed version reflection spectrum of wavelength shift

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 12. Then it can be easily translated into ASCII format which will be used for fabrication. The GDSII file as shown in figure 4was then verified with respect to its rulings with the help of K-layout tool and it is shown in Fig 13.

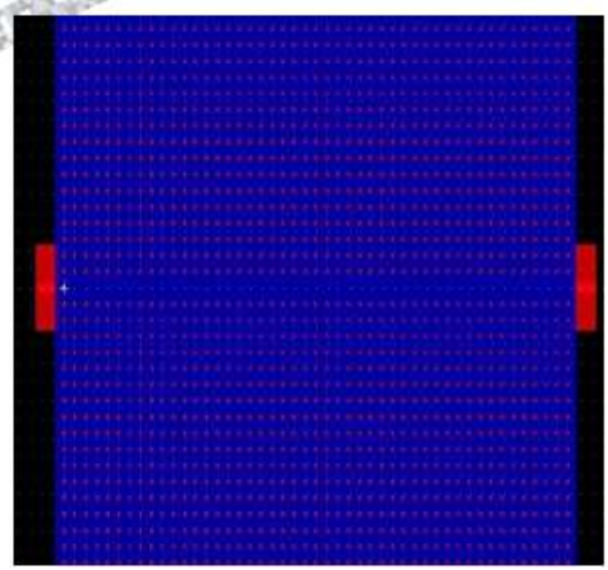


Fig. 12: GDSII file from OWLVISION (GDS viewer tool)

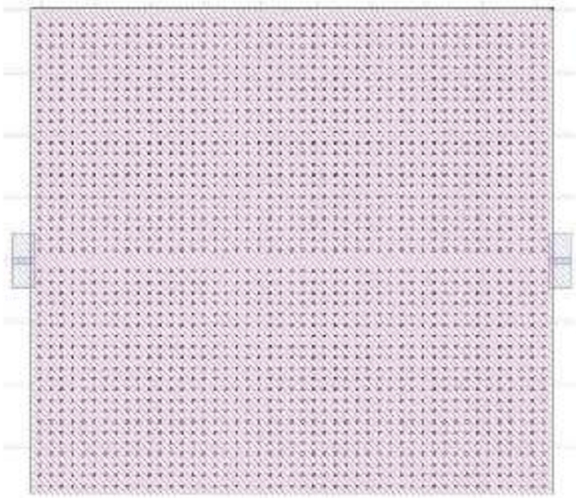


Fig. 13: GDSII file from K-layout

Table 1: shifts in frequency and wavelength spectrum

	Frequency spectrum (normalized)		Wavelength spectrum(um)	
	trans mission	refle ction	trans mission	reflecti on
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.

CONCLUSION

Photonic biosensors based on evanescent wave detection have demonstrated its outstanding properties, such as extremely high sensitivity for the direct measurement of bimolecular interactions, in real–time.

The sensor design consists of a two dimensional square lattice line defect photonic crystal structure. Using Photonic Crystal the impact of fluoride with respect to refractive index & wavelength shift is observed. Photonic crystal based biosensor is used as design. The results in MEEP are obtained. 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.

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