Design and Simulation of a Photonic Crystal Based Optical Sensor for Detecting Ammonia using Transmission Spectrum Analysis

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***Abstract*—Ammonia is a useful chemical. It is used in manufacturing fertilizers and various other industries. But it can be hazardous to human beings, when in higher concentration in air. Also, it is highly toxic to aquatic animals, even at dilute concentration. This has an indirect effect on human beings. Therefore, it is considered dangerous for the environment. In this paper, a design of an optical sensor based on photonic crystal is proposed. Photonic Crystals are materials of periodic structure that have effects on light beams when incident or pass through it. Photonic crystals are analogous to semiconductors in the sense that the lattice can prohibit the propagation of certain waves. There may be gaps in the energy band structure of the crystal called photonic band gaps similar to those in semiconductors. Different structures can be made using these crystals such as cavities, waveguides, ring resonators etc. These structures along with appropriate light source can be used as sensors for different chemicals by using those chemicals in the background due to the fact that, when the refractive index of the respective chemical is different, there is a change in resonant wavelength and transmission spectrum. Ring resonator based structure and rods in air configuration are used in the design. Analysis method employed is FDTD (Finite difference time domain) and the MEEP (MIT Electromagnetic Equation Propagation) is the tool used to model and design the structure. Transmission flux levels, sensitivity and Q-factor are the parameters studied.**

***Index Terms*—Ammonia, FDTD, sensor, photonic crystal, ring resonator.**

I. Introduction

As the word suggests, ‘photonics’ is derived from the Greek word ‘photos’ which means light. It is said that photonics as a field began with the invention of laser in 1960. Some of the areas that have emerged since the beginning are bio-photonics, Nano-photonics, silicon photonics, plasma photonics, terahertz photonics, microwave photonics, integrated photonic systems[1].

Photonic crystals are materials of periodic structure that have effects on light beams when incident or pass through it. Photonic crystals are analogous to semiconductors in the sense that the lattice can prohibit the propagation of certain waves. There may be gaps in the energy band structure of the crystal called photonic band gaps similar to those in semiconductors[2]. Studying photonic crystals involves a study of combination of solid state physics and electromagnetics. Photonic crystals can be found in nature. Examples for naturally found photonic crystals are peacock feather and wings of the butterfly. They can be also be created artificially. There are various types, shapes and structures of artificiallycreated photonic crystals. One such classification is in the dimensionality. 1d,2d and 3d photonic crystals have been fabricated in labs. [3]

II. Defect Engineering

A defect in a photonic crystal can be absence of one or more layers, rods or holes in the periodic structure or it can be variation of the usual structure that is repeated inside the crystal such as change in size of radius of a rod or hole. When a defect is introduced in the photonic crystal structure, the forbidden wavelength may occupy or pass through the defect. They include point and line defects. When light is incident upon the point defect, then light is prevented from entering the surrounding structure and is reflected back at a timely basis. The point defect acts like a cavity. This is similar to resonance in electronic circuits. A series of point defects can be introduced to form a line defect. Light beam entering from one end of the line-defect, will cause light of forbidden wavelengths (in band gap) to take only the path of that line, as it is forbidden from going into any other paths containing periodic structure. A line defect guides the wave and hence it is nothing but a waveguide. Defect engineering involves creating various structures using these defects in a photonic crystal. Defect engineering has resulted in design of complex structures and has proved to be an useful and interesting area of research.

Refractive index based photonic crystal sensors make use of the fact that property of light changes due to change in refractive index. Most of the advanced sensor architectures use refractive index sensing for detection. Two primary types of sensing mechanism are surface sensing and homogeneous sensing. Surface sensing involves target molecules being made to be adsorb on suitable receptors. Photonic crystal holes act as surface for receptors. Local refractive index changes when molecules from the sample are adsorbed on these receptors. In homogeneous sensing, the effective refractive index of the fiber varies due to variation in the refractive index of the cover resulted from gas and liquid samples [4].

Following are some of the advantages of using photonic

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crystal based sensors for detecting chemicals: selectivity and sensitivity obtained are high;the chip promotes parallel processing; wavelength readout (noise and interference immunity); low-cost and high integration with front-end and support electronic systems;real-time processing [5].

Two important parameters that are considered to evaluate the performance of these sensors are: 1.Sensitivity and 2.Quality factor. Sensitivity is defined as the ratio of change in resonant wavelength($\Delta\lambda$) to change in background refractive index (Δn).

$$S_\lambda=\Delta\lambda/\Delta n \quad (1)$$

Quality factor defines the resonant peak and is given by

$$Q=f_0/\Delta f \quad (2)$$

III. FDTD AND MEEP

Finite-difference time-domain, FDTD is one of the most common algorithms used to compute electromagnetic fields. It divides space and time into a regular grid and simulates the time evolution of Maxwell's equations.[6] Maxwell's Equations in Point Form (Differential Form) Time Domain are given below from (3)-(5).

$$\nabla\times E=-\partial B/\partial t \quad (3)$$

$$\nabla\times H= (\partial D/\partial t) +\text{"J"source} \quad (4)$$

$$\nabla . B=0 \quad (5)$$

$$\nabla . D=0 \quad (6)$$

where

E = V/m = N/C,Electric Field

D = C/m^2,Electric Flux Density

H = A/m, Magnetic Field

B = Wb/m^2 = Tesla = N/(A*m),MagneticFlux Density

q_v = C/m^3, Charge Density (volume)

J = A/m, Current Density

By substituting $\delta /\delta t = 0$ in above equations, we get the static form.

Consider the two equations given below:

$$\nabla\times E=-\mu(\partial H)/\partial t \quad \text{(nomagneticloss)}$$

$$(7)\nabla\times H=\sigma E+\varepsilon(\partial E)/\partial t \quad (8)$$

To obtain FDTD equations from the above two equations

i. The vector equations are converted to scalar equations by computing thedeterminants (curl of the respective vectors) .

ii. The scalar differential equation is then converted to scalar difference equation by considering the Yee grid[18] shown in the Fig 1.

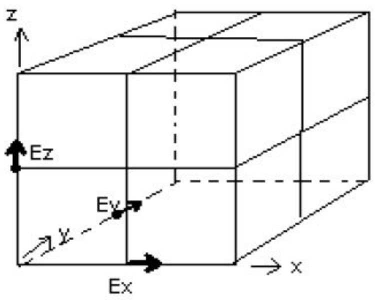

Fig 1: Yee grid

The flowchart of the FDTD algorithm [18] in a simple form is shown in Fig 2. First electric and magnetic fields, E and H are set to 0 as initial conditions. Then the sources are considered. Next, electric fields are calculated using the Maxwell's equations and Yee lattice. Then magnetic fields are calculated from the previously calculated electric fields. Again, the electric fields are update with the help of sources and previously calculated magnetic fields. These steps are repeated till final time step is reached.

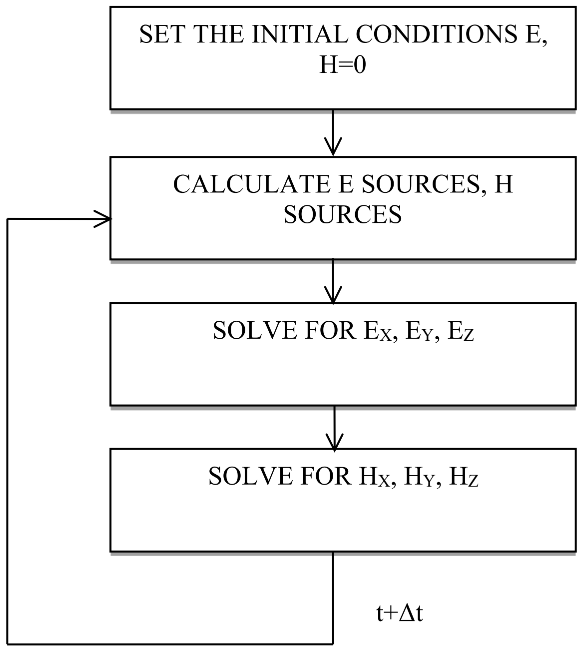

Fig 2: Flowchart of FDTD algorithm

In its official website, MEEP is defined as follows: Meep (or MEEP) is a software tool used to model electromagnetic systems such as photonic crystals. It uses finite-difference time-domain (FDTD) algorithm. The full form of Meep is MIT Electromagnetic Equation Propagation [7].The program file of Meep is a control file with an extension ".ctl". Geometry, current sources, outputs computed, and

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everything else specific to the required calculations are specified in ctl file. The ctl file is written in a scripting language.MEEP can be used to design and implement the photonic crystal structures, and to obtain transmission, reflection spectrums and other important parameters.

IV. AMMONIA AND ITS DETECTION

Ammonia is a useful chemical. It is used in manufacturing fertilizers and various other industries. But it can be hazardous to human beings, when in higher concentration in air. Toxicological profile for ammonia published by U.S. department of health and human services public health service agency for toxic substances and disease registry discusses the health effects of ammonia exposure on humans. Exposure to ammonia causes death when acute exposures of 5000 to 10000 ppm occur. These exposures happen due to accidents. Other effects of inhalation exposure include respiratory effects such as irritation to nose and throat,breathing difficulties; cardiovascular effects which include elevated pulse and blood pressure, bradycardia, and cardiac arrest in humans and gastrointestinal effects like burns of the lips, oral cavity, and pharynx, along with edema of these areas. Other effects include hematological effects, musculo-skeletal effects, hepatic effects, endocrine effects, dermal effects, ocular effects and neurological effects. Also, it is highly toxic to aquatic animals, even at its presence in dilute concentration. Concentrations of ammonia in water can cause loss of equilibrium, hyper-excitability, increased breathing, cardiac output, and oxygen uptake in fishes, and, in extreme cases, convulsions, coma, and even death. At lower concentrations, ammonia produces many effects in fish including a lower egg hatching success, a lower growth rate and morphological development, and alarming changes in the tissue of the gills, liver and kidney[8],[9].

Ammonia, when in smaller concentration, can be detected chemically using Nessler's solution or due to the smell when warmed with quicklime. Electrochemical and holographic techniques have been used to detect ammonia in higher concentrations. These techniques need chemicals and heavy equipment for detection. So, photonic crystal is a viable option.In the past, many compact sensors have been designed to detect ammonia. Karasinski et.al have fabricated planar evanescent wave ammonia sensor using sol-gel technology.[10] An optical sensor for gaseous ammonia with tuneable sensitivity was fabricated by Teresa Grady et.al. [11]. Kuchyanov et.al have fabricated a highly sensitive ammonia sensor using reflection of light at a glass[12].Selective and reversible ammonia gas detection with functionalized silicon-on-insulator optical micro-ring resonators has been demonstrated by Nebiyu A. Yebo et.al[13].In this project work a photonic crystal based ring resonator shall be used to detect ammonia. The output transmission flux of a photonic crystal structure changes due to change in refractive index of the defect. Different refractive indices give different transmission spectrum. Hence these distinct spectrums can be analyzed and the differences can be observed to detect presence of ammonia.

V. DESIGN

The design and simulation is done with the help of MEEP tool. The papers related to photonic crystal based sensors have been analyzed to note that different parameters that have been used [14]-[17]. So, many different design parameters were tested and the following were selected for the implementation:

1)Rods in air configuration
2)Square lattice structure
3)Lattice constant 'a'=1μm
4)Radius of rods 'r'=0.2μm
5)Dielectric constant of silicon rods =12
6)Dielectric constant of back ground is changed with respect to different chemicals
7)Source used is Gaussian in nature

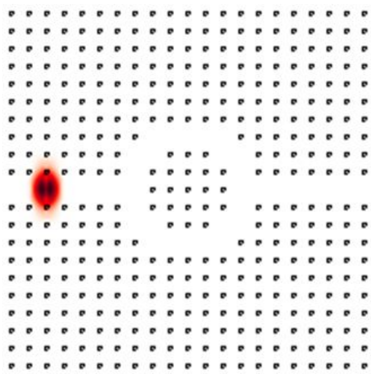

Fig 3: The hybrid ring resonator structure used for detecting Ammonia

The structure shown in fig 7.2 is a hybrid ring resonator. A square cell of size 21X21 is created first. A basic rod of silicon is formed at the center and then it is duplicated in both x and y direction to get the square array of rods. First the left and right line defects are created by changing the refractive index or dielectric constant of the rods in those lines. Next the circular defect is created by the same process of changing dielectric constant of appropriate rods. The source is placed at left end of the structure and output flux is measured at the left end.

VI. RESULTS

The structure shown in Fig.3 is used as the detecting device. To detect ammonia in air, transmission spectrums when air and gaseous ammonia are used in the background, are obtained. Similarly transmission spectrums of liquid ammonia and water are obtained by using them in the introduced defects, to detect ammonia in water. MEEP provides the frequency and the output transmission flux as well as harminv values. Number of frequencies where output flux had to be evaluated was 500 (nfreq=500). All the 500 values got through MEEP are imported to an excel sheet. The values in excel sheet are then imported to MATLAB and are plotted using MATLAB.

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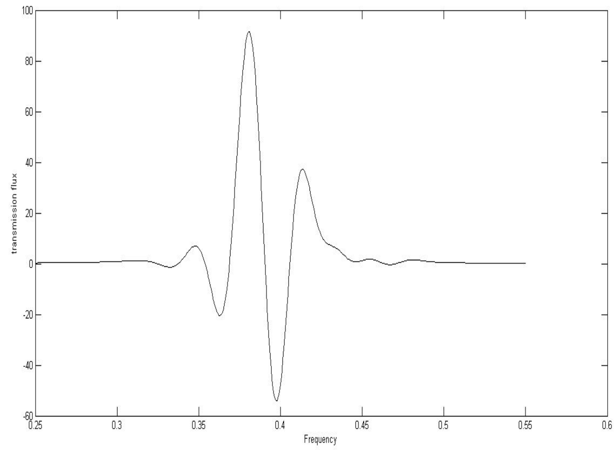

Fig 3: The graph of output transmission flux versus frequency when air is used in the background

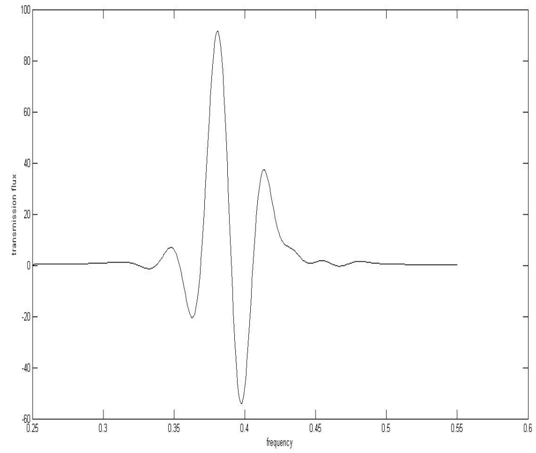

Fig 4: The graph of output transmission flux versus frequency when gaseous ammonia is used in the background

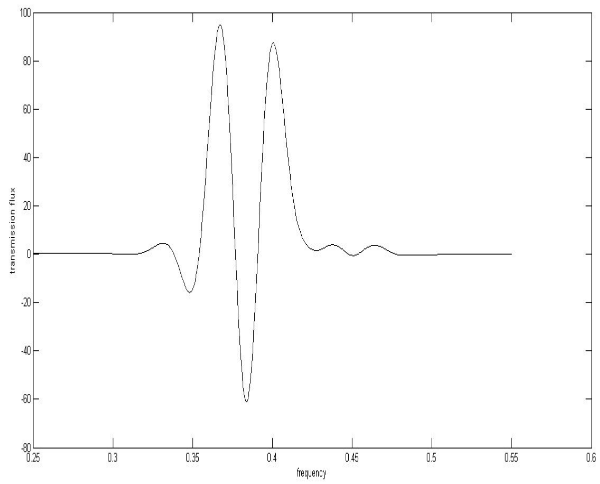

Fig 5: The graph of output transmission flux versus frequency when water is used in the background

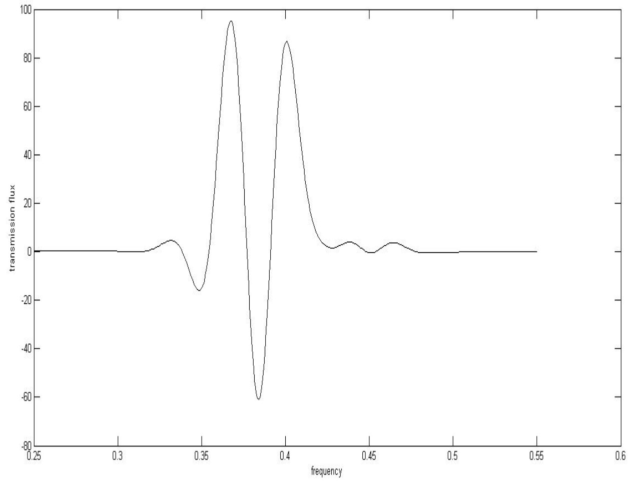

Fig 6: The graph of output transmission flux versus frequency when liquid ammonia is used in the background

The graph shown in Fig 3 was obtained when air (refractive index = 1) was used as the background chemical in the defect. The source was placed at the left end of the structure at coordinates (-8, 0) and flux region at the right end at (8,0). The graph of output transmission flux versus frequency shown in fig 4 is the one got when gaseous ammonia (refractive index= 1.00267) is used in the defect.it may look similar to the one in Fig 3.This is because the difference between refractive index of gaseous ammonia and air is very small But when zoomed, a difference can be seen. This difference can be analyzed to detect ammonia present in air. When water (refractive index= 1.33) is used in the defect, the graph of output transmission flux versus frequency shown in Fig 5 is obtained. The source and flux region are placed at the same points as mentioned earlier The graph of shown in fig 6 is the one obtained when liquid ammonia (refractive index= 1.325) is used in the defect. A clear difference between Fig 5 and Fig 6 can be seen. This difference is analyzed to detect ammonia present in water.

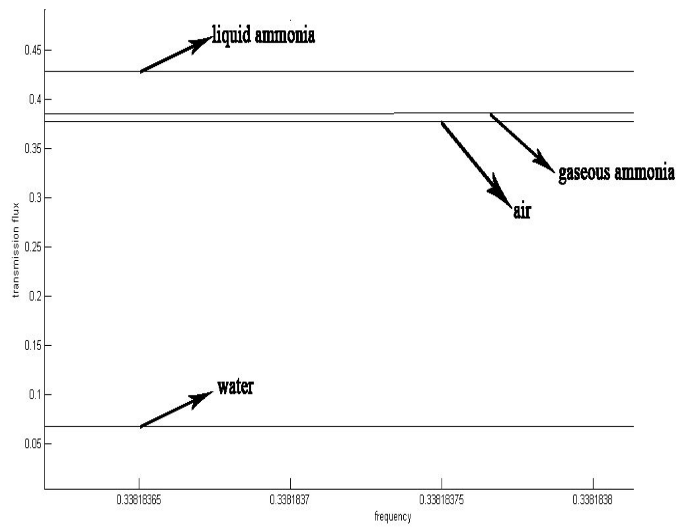

Fig 7: A zoomed version of the graph of combined output transmission flux versus frequency when 4 different chemicals are used in the background

The graph in Fig 7 showsa zoomed version of the graph of combined output transmission flux versus frequency. It can be observed that for a certain frequency range the

ISSN: 2278 – 7798

transmission plots are distinct for all the chemicals used in the background.

The sensitivity was calculated using the equation (1). It is obtained to be 172.5nm/RIU. The Q- factors obtainedare tabulated as shown in Table I.

Material	Q-factor
Air	101
Gaseous ammonia	135
Water	3347
Liquid ammonia	6658

Table I

VII. Conclusion

In this work, a photonic crystal based sensor has been designed. The output transmission flux was obtained when air, water liquid and gaseous ammonia were used in the background. Since the difference between refractive indices of air and gaseous ammonia is small, the flux spectrums looked similar but a zoomed version verifies that there is a clear distinction in the spectrum. But for water and liquid ammonia, there is a clear distinction. The transmission spectrum obtained from the simulation shows distinct shifts in frequency and wavelength. Change in the transmission flux is observed for different chemicals. The sensitivity obtained was 172.5nm/RIU. This design provides a miniaturized, cost effective, low energy sensor system[4].

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