Simulation Design of Hollow Core Photonic Crystal fiber for Sensing Water Quality

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Abstract. In this work we submit a simulation design to sense the water quality using hollow core photonic crystal fiber. The work of this types of optical fibers depending on the variety of structural design and geometrical parameters. The numerical results are studied by using the Finite Element Method (FEM) through COMSOL MULTIPHYSICS simulation software. Different concentrations from (0%) to (100%) of D2O and H2O2 solution in water as sensed liquid had been chosen. The studied HC-PCF investigated for analyzing the relative sensitivity, effective area and confinement loss at wavelength range from (1) μm to (2) μm.

1. Introduction

One of the worst sides of manufacturing factories is the wastes by-products on the environment, where wastewater made by industrial activities consider as a major cause to water pollution in the world due to the many amounts of chemical producers used in the processes. Such wastewaters are liberal with chemical remains containing heavy metal and coloring and sometimes without color like the addition of H2O2 (hydroperoxide) to the water with 50% it will consider the water as toxic also with D2O (deuterium peroxide), so it's important to design a sensor for this type of water [1]. Photonic Crystal Fibers (PCFs) are a new advanced type of optical fiber which made from a single dielectric material. The cladding area of PCF consist of air holes organized in 2D array patterns [2]. The PCFs invented by Russel et al. and its companion nearly 1996 made these type of optical fiber had the flexibility in design to be used in many fields like communication, sensing and detection among many other, so from that time the researchers depending on that flexibility in design to study a numerous structural diversity of PCFs [3], figure 1, shows some types of PCF’s. The work of PCF depending on the variety of structural design and geometrical parameters which depend on the diameters of both the core (D) and the air holes (d) and the spacing between the two centers of contiguous air holes (A). These factors made the properties of PCF like briefings, endlessly single mode, polarization, confinement loss and sensitivity [4]. Due to the kind of the core, PCF can be labeled into two types: (1) Solid Core – Photonic Crystal Fiber (SC-PCF) which using the modified total internal reflection as a light guiding mechanism, and (2) Hollow Core – Photonic Crystal Fiber (HC-PCF) which using the photonic band gap effect as a light guiding mechanism. Every type of the previous types has unlimited designs and every design had the specific application to use in [5] figure 2, shows the above two types of PCF’s.
In this paper, new designs of HC-PCFs were presented as a water quality sensor with high sensitivity depending on the affected mode area where the sensing material interact with the light and made the fundamental mode among other factors. The numerical results are studied by using the Finite Element Method (FEM) through COMSOL MULTIPHYSICS simulation software. The concentration range had been chosen from (0%) to (100%) of D$_2$O and H$_2$O$_2$ solution in water as sensed liquid. The refractive indexes of D$_2$O and H$_2$O$_2$ solution concentrations for are calculated in wavelength 1.55 μm. The studied HC-PCF investigated for analyzing the relative sensitivity, effective area and confinement loss at wavelength range from (1) μm to (2) μm.

2. Experimental Work

A circular hollow core PCF consist of hollow core with diameter ($D_{core}$=7.6μm) and 3 ring of air holes around, every ring with 24 air holes arranged in circular style with diameter of (1.56,1.6, and 1.7 μm respectively) had been designed. The spacing between the core and the first ring equal to (6μm) and the pitch between the air holes equal to (2μm) the air holes rotate by an angle equal to (15°). The outer cladding with diameter of (26.6 μm) with PML layer (Perfectly Mach Layer). The dielectric material of the fiber is pure silica and the air holes filled with water at the first time with refractive index ($n_{H2O}$=1.333), the with H$_2$O$_2$ (Hydro-peroxide) with refractive index ($n_{H2O2}$=1.4060), and at last with D$_2$O (deuterium peroxide) with refractive index ($n_{H2O}$=1.328), then filled the air holes with different concentration mixed with water in range of wavelength of (1-2)μm. Figure 3 shows the cross section of the submitted HC-PCF.

For studying the behavior of the studied PCF numerically we used a method called Finite Element Method (FEM). This method is one of many methods for numerical study like Time Domain Method.
(FTDTM) and Effective Index Method (IEIM), here used to analyzing the electromagnetic propagation in PCF also for accruing the resultant. Silica is used as a background material of PCF for its unique optical properties and it consider as a background material. The refractive index (RI$_i$) of silica is calculated by Sellmeier equation [6], as in Eq. (1)

$$n^2 - 1 = \sum_{i=1}^{3} \frac{B_i \cdot \lambda^2}{\lambda^2 - C_i^2} \ldots \ldots \ldots \ldots \ldots (1)$$

Where $B_i$ and $C_i$ are the coefficients related to the material and temperature. For Si

$B_1 = 6.96166300 \times 10^{-1}$ \hspace{1cm} $C_1 = 4.67914826 \times 10^{-3}$ \mu m$^2$

$B_2 = 4.07942600 \times 10^{-1}$ \hspace{1cm} $C_2 = 1.35120631 \times 10^{-1}$ \mu m$^2$

$B_3 = 8.97479400 \times 10^{-1}$ \hspace{1cm} $C_3 = 9.79340025 \times 10^1$ \mu m$^2$

Like silica the refractive index of water (H$_2$O) could be calculated from eq.1 but $i$=1 to 4 limits so eq.1 will be [7]:

$$n^2 - 1 = \sum_{i=1}^{4} \frac{B_i \cdot \lambda^2}{\lambda^2 - C_i^2} \ldots \ldots \ldots \ldots \ldots (2)$$

Where $B_i$ and $C_i$ for H$_2$O:

$B_1 = 5.689093832 \times 10^{-1}$ \hspace{1cm} $C_1 = 5.110301794 \times 10^{-3}$ \mu m$^2$

$B_2 = 1.719708856 \times 10^{-1}$ \hspace{1cm} $C_2 = 1.825180155 \times 10^{-2}$ \mu m$^2$

$B_3 = 2.062501582 \times 10^{-2}$ \hspace{1cm} $C_3 = 2.624158904 \times 10^{-2}$ \mu m$^2$

$B_4 = 1.123965424 \times 10^{-1}$ \hspace{1cm} $C_4 = 2.624158904 \times 10^1$ \mu m$^2$

While the refractive index of both Hydro-peroxide and Deuterium peroxide are taken from references [8] and [9] respectively.

The confinement loss, $L_c$ could be calculated by using the imaginary part of the complex effective index $n_{eff}$ through the spread constant of the leaky optical mode from the core into the outer air hole region in studying a finite number of layers of air holes, by using the following Eq. (3) [10]:

$$L_c \left[ \frac{dB}{m} \right] = 8.686 * k_o * l_o [n_{eff}] \ldots \ldots \ldots \ldots \ldots (3)$$

Where $k_o$ the wave number in the vacuum which equal to $(2\pi/\lambda)$ where (\lambda) the wavelength, $l_o[n_{eff}]$ is the imaginary part of the effective mode index.

The area where the interaction between light and the sensed material and the parameter affected the relative sensitivity. The effective area could be calculated through eq.4 [11]

$$A_{eff} = \frac{\left( \int \int |E_{(x,y)}|^2 \, dx \, dy \right)^2}{\int \int |E_{(x,y)}|^4 \, dx \, dy} \ldots \ldots \ldots \ldots \ldots (4)$$

Where $E$ is the electric field vector

The value of intensity of confined light largely dependent on nonlinear coefficient ($\gamma$) of the studied PCF and represent the Eigen modes and could calculated by using eq.5 [12]
\[ r = \frac{n_r}{n_{eff}} \times f \]  

The interaction between light and the sensed material could be showed in Beer-Lambert Law which is related to the relative sensitivity \( r \) coefficient at a specific wavelength. It can be calculated through the following Eq. (6) [13]

\[ r = \frac{n_r}{Re[n_{eff}]} \times f \]  

Where \( n_r \) is the refractive index of sensed material in the air holes and \( n_{eff} \) is modal effective index, and, \( f \) is the percentage ratio of the air hole power which expressed as eq.7

\[ r' = \frac{\int_{sample} Re[H_x H_y - H_y H_x] dx dy}{\int_{total} Re[H_x H_y - H_y H_x] dx dy} \times 100 \]  

Where \( E_x, E_y \) and \( H_x, H_y \) are the transverse electric fields and magnetic fields of the fundamental propagating mode. The ratio \( f \) defines the percentage of energy present in the holes.

### 3. Results and Discussion

In this part, the numerical study will be discussed for the studied HC-PCF in fundamental mode on some expansion characteristics of Water, D2O, and H2O2 have been chosen for filling the core and the air holes. The simulation has been operated actively at a wide range of wavelengths from 1 μm to 2 μm. Figure 4 shows the fundamental mode for selective wavelength.

![Figure 4. Intensity distribution for selected mode Modal.](image)

At first step we analyzed the effective index \( n_{eff} \) of the liquids infiltrated in the PCF core and air hole. The behavior of \( n_{eff} \) versus wavelength range shown in figure 5, which represent the \( n_{eff} \) of water and D2O and figure 6, which represent the \( n_{eff} \) of water and H2O2, shows the behavior of \( n_{eff} \) of the infiltrated PCF at different wavelengths. It showed that with increasing the operating wavelength there are a linear decrease in effective indices for water, D2O and H2O2 respectively, which consider as a normal behavior for \( n_{eff} \).

To analyze the relative sensitivity of H2O2 and D2O solutions, effective area \( A_{eff} \) as well as confinement loss \( L_c \) of the studied HC-PCF structure which were calculated from eqs. 6,4 and 3 respectively. The PCF core region is filled with different concentrations solution of H2O2 and D2O in water. For each amount of concentrations of H2O2 and D2O solutions, the simulation is computed at wavelength 1.55 μm. We nots from figure 7, that the relative sensitivity decreasing by increasing of concentration and its variation between 97% to 67% for H2O2 solution while it’s between 80% to 41% for D2O where the relative sensitivity dependence on effective refractive index profile.
4. Conclusions

New design of HC-PCFs were presented as a water quality sensor. The numerical results are studied using the Finite Element Method (FEM) through COMSOL MULTIPHYSICS simulation software. The concentration range had been chosen from (0%) to (100%) of D_2O and H_2O_2 solution in water as sensed liquid. The studied HC-PCF investigated for analyzing the relative sensitivity, at wavelength range from (1) μm to (2) μm. The submitted design had a very good sensitivity which make it a very good element to detect the water pollutant and to measure water quality.
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