Terahertz detection of alcohol using a photonic crystal fiber sensor

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Ethanol is widely used in chemical industrial processes as well as in the food and beverage industry. Therefore, methods of detecting alcohol must be accurate, precise, and reliable. In this context, a novel Zeonex-based photonic crystal fiber (PCF) has been modeled and analyzed for ethanol detection in terahertz frequency range. A finite-element-method-based simulation of the PCF sensor shows a high relative sensitivity of 68.87% with negligible confinement loss of $7.79 \times 10^{-12} \text{ cm}^{-1}$ at 1 THz frequency and $x$-polarization mode. Moreover, the core power fraction, birefringence, effective material loss, dispersion, and numerical aperture are also determined in the terahertz frequency range. Owing to the simple fiber structure, existing fabrication methods are feasible. With the outstanding waveguiding properties, the proposed sensor can potentially be used in ethanol detection, as well as polarization-preserving applications of terahertz waves.

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1. INTRODUCTION

Photonic crystal fiber (PCF)-based sensors are significant because of their high relative sensitivity, small size, flexibility, and robustness. In a PCF, characteristics such as relative sensitivity, core power fraction, effective material loss (EML), birefringence, dispersion, etc., can be engineered by optimizing the shape and position of air holes, core diameter, diameter of the air holes used in both the core and cladding, and the pitch (distance between two consecutive air holes), which is difficult to achieve using conventional optical fiber [1]. Moreover, PCF is robust to environmental conditions such as strong electromagnetic fields, noise, high voltages, chemically corrosive environments, and high temperatures. The existence of air holes in both the core and cladding of a PCF allows guided transmission of light through them and provides the ability to insert analytes (gases, chemicals, etc.) into the air holes, facilitating confined interaction of light with the sample, leading to new sensing applications [2].

We focus this study on ethanol, being a common form of alcohol used in both industrial processes and in the beverage industry. There are several methods to quantify the amount of alcohol in beverages that include physical (densitometry, pycnometry, and hydrometry), chemical (dichromate oxidation), spectrometric, and chromatographic analyses [3]. A number of studies have been carried out for ethanol detection in recent years. In 2006, Xu et al. proposed ZnO nanorods for detecting ethanol. They used a hydrothermal process with zinc powder and cetyltrimethylammonium bromide (CTAB) at 182°C [4], but this high temperature limits practicability. Later, for ethanol detection in alcoholic beverages, Shkotova et al. proposed an amperometric bio-sensor [5]. They used Resydrol polymer to detect the ethanol. A graphite epoxy composite electrode (GECE)-based bio-sensor was then proposed by Kirgöz et al. [6]. They claimed that their designed bio-sensor is a practical and economic tool for detecting ethanol and aspartame in real samples. In 2007, to quantify the ethanol concentration in alcoholic beverages, Raman spectroscopy was introduced [7]. For air pressure sensing applications, a numerical study on a highly birefringent microstructured PCF was demonstrated by Jewart et al. [8]; however, their obtained birefringence was relatively low at 0.0011. Recently, an optical-fiber-based sensor coated with polypyrrole-polyethylene oxide (PPO) material was investigated to detect volatile compounds such as ammonia, triethylamine, methanol, ethanol, and acetone vapors [9]. In 2016, Isaac-Lam proposed a 45 MHz benchtop nuclear magnetic resonance (NMR) spectrometer for the detection of alcohol content in alcoholic beverages [3], but the obtained spectral resolution is low because of the low operating frequency.
In 2016, an elliptical air-hole-based hybrid core PCF-based chemical sensor was proposed [10]. Tuning their designed sensor, they obtained a relative sensitivity of 49.17% with a low birefringence of 0.0015. Later, to increase the sensitivity, Arif et al. [11] proposed a sensor with a different air hole diameter. In that way, they obtained a relative sensitivity of 59%. Moreover, in recent years, a number of PCF-based sensors were also proposed for chemical analyte detection [12–16]. However, using silica as the background material, all the previously proposed PCF-based sensors were designed to operate in the optical wavelength region.

Thus, there is a large scope for development of a PCF-based sensor that operates at terahertz frequencies in order to obtain a diverse range of application. The optical wavelength region (100 nm to 1 μm) is a well-developed technology. However, for fluid sensing with porous fibers, (i) terahertz components are easier to manufacture compared to those in the optical regime, and (ii) molecular resonances tend to be in the terahertz range, making it an ideal candidate for chemical sensing. As an advancement of terahertz technology, different types of terahertz functional devices such as terahertz absorbers [17–19] and terahertz directional couplers [20] have been developed. Moreover, dielectric tube [21] and PCF-based waveguides [22,23] have also been introduced for terahertz wave transmission.

There are several polymers that can be used as a background material of a terahertz PCF-based sensor. The most commonly used polymer materials are polytetrafluoroethylene [24], polyethylene (HDPE) [25], polymethyl-methacrylate (PMMA) [26], Teflon [27], Cyclic-Olefin Copolymer (COC) [22,23,28], and Cyclo-Olefin Polymer (COP) [29]. We used COP commercially named as Zeonex as the background material because of its lower material absorption loss than other polymer materials (0.2 cm\(^{-1}\) in terahertz frequency range), constant index of refraction of 1.53 (and as such, the material dispersion is negligible), negligible water absorption (<0.1%), high transparency, high glass transmission temperature, and excellent optical stability, even after heat and humid exposure [29–31].

In this paper, to the best of our knowledge, for the first time in the research of optical sensors, we introduce a PCF-based terahertz sensor mainly for alcoholic beverages detection. In a Zeonex substrate, we introduce an array of elliptical air holes in a modified hexagonal lattice structure. Besides high sensitivity, the reason for using elliptical shaped air holes inside the core is to make the sensor qualified to work on polarization-maintaining applications of terahertz waves. The aim is to make the sensor applicable not only in alcohol detection but also in the field of biomedical imaging and polarization-maintaining applications of terahertz waves.

2. PHYSICAL ARCHITECTURE OF THE PROPOSED PCF-BASED TERAHERTZ SENSOR

The physical architecture of the proposed terahertz sensor is shown in Fig. 1. Finite-element-method-based commercially available software COMSOL v. 4.3b was used for modeling and numerical simulation of the sensor. Our approach may be extended to other types of liquid by inserting the characteristics of those liquids in the material section of COMSOL.

As shown in Fig. 1, the air hole diameters in the cladding region are all kept the same, denoted as \(d\). The distances of the air holes in the cladding region that lie in the same ring and immediate next ring are denoted by \(A\) and by \(A_1\), respectively. In order to increase the sensitivity, we design the air hole size inside the core to be as large as possible. This is because as the air hole size increases, the amount of ethanol filled inside the air hole also increases, which consequently increases light-matter interaction. As the level of light-matter interaction (core power fraction) is proportional to sensitivity [refer to Eq. (3)], consequently increased core power fraction increases the relative sensitivity. Also, elliptical shaped air holes are used inside the core so that the proposed PCF can also be applicable in polarization-maintaining applications of terahertz waves. Inside the elliptical shaped air holes, we used ethanol as the analyte with refractive index 1.354. The main goal is to detect ethanol as a primary form of alcohol. The width and length of the elliptical air holes inside the core are denoted as \(W_c\) and \(L_c\). During the numerical simulation, we keep the length of each air hole fixed, while the width is varied. Keeping the length \(L_c = 147 \mu m\) the same, we vary the width of \(W_c\) to 36 μm, 38 μm, and 40 μm. The total fiber diameter is 3.2 mm. In Fig. 1, \(D_{core}\) indicates the core region of length \(L = 890 \mu m\) and width \(W = 220 \mu m\), which are kept fixed throughout the whole numerical simulation. The center-to-center air hole distances in horizontal and vertical directions of the core region are denoted as \(p_x\) and \(p_y\). We keep the air filling fraction (AFF) at the cladding region fixed at 0.94 because further increase may be the cause to overlap the air holes with each other, and that may create the fabrication difficulties. Perfectly matched layer (PML) absorbing boundary conditions were used to control the outgoing waves from the fiber. The thickness of the PML boundary was only 10% of the fiber radius. In choosing the PML thickness, we followed the convergence test result carried out in our previous publication [23]. In Ref. [23], it can be seen that variation of PML thickness does not affect the real part of the complex refractive index. As only the real part of the refractive index is required for measuring the relative sensitivity [as mentioned in Eq. (3)] and also considering the fabrication effectiveness as mentioned in Ref. [23], we choose such PML thickness.

The relative sensitivity of a terahertz fiber sensor can be calculated via the intensity of light-matter interaction. This is dependent on the absorption coefficient at a particular frequency. According to the Beer–Lambert law [11],

\[
\text{Relative Sensitivity} = \frac{I_0}{I} = \exp(-\alpha L)
\]
\[ I(f) = I_0(f) \exp[-ra_n f l], \]  
\[ A = \log \left( \frac{I}{I_0} \right) = -ra_n f l. \]  
\[ r = \frac{n_r}{n_{eff}} \times \varepsilon, \]  
where \( r \) denotes the relative sensitivity, \( n_r \) represents the refractive index of the analyte needed to be detected (which is 1.354 in the case of ethanol), \( n_{eff} \) denotes the effective refractive index of the guided mode, and \( \varepsilon \) is the amount of light-matter interaction, which can be calculated by [13]
\[ e = \frac{\int_{\text{sample}} R_h(E_x^2 H_y - E_y^2 H_x) \, dx \, dy}{\int_{\text{total}} R_h(E_x^2 H_y - E_y^2 H_x) \, dx \, dy} \times 100, \]  
where \( E_x, E_y, H_x, H_y \) are the electric field and magnetic field components of the guided modes, respectively.

Characterization of dispersion properties will help to examine the fiber’s ability to operate for multichannel communication application. In Zeonex, the material dispersion is negligible, so it is necessary to calculate only the waveguide dispersion of the proposed PCF. Waveguide dispersion of a fiber can be calculated by [35]
\[ \beta_2 = 2 \frac{dn_{eff}}{d\omega} + \frac{w d^2 n_{eff}}{c d\omega^2}, \text{ ps/THz/cm}, \]  
where \( \beta_2 \) indicates the dispersion parameter, \( \omega = 2\pi f \) indicates the radian frequency, \( c \) is the speed of light into free space, and \( (n_{eff}) \) represents the effective refractive index of the proposed waveguide structure.

The area covered by the interaction of light intensities with matters can be calculated by the term effective area. A higher modal effective area is suitable for laser and communication devices, whereas a lower modal effective area is suitable for nonlinear effects [36]. It can be characterized by [35]
\[ A_{eff} = \frac{\left( \int |I(r)| \, dr \right)^2}{\int |I^2(r)| \, dr}, \]  
where \( A_{eff} \) represents the area covered by the guided modes, and \( I(r) = |E_z|^2 \) is the transverse electric intensity distribution throughout the cross section of the fiber.

For broad sensing application, a wide numerical aperture (NA) is desirable and is achieved when the refractive index difference between the core and cladding of a PCF can be made larger. Note that NA can be quantified by the following equation [37]:
\[ \text{NA} = \frac{1}{\sqrt{1 + \frac{\pi A_{eff} f_z^2}{c^2}}}, \]  
where \( A_{eff} \) represents the effective area of the proposed PC-PCF sensor.

3. Fabrication Possibilities of Elliptical Array Shaped Core Hexagonal-Clad PCF Sensor

In order for the proposed PCF fiber to have practical applications, including industrial and commercial sensing, it must be manufacturable. The proposed PCF consists of a hexagonal structure with all circular shaped air holes in the cladding and array of elliptical air holes inside it. The circular shaped air hole structures can be readily fabricated using the stacking and drilling method [38,39]. Moreover, the sol-gel [40] technique can also be used to fabricate circular shaped air holes.
Fabrication of elliptical shaped air holes is easily possible using the existing fabrication technologies. There are a number of studies with fabricated elliptical shaped air holes [41–46]. Using monomer polymerization, elliptical shaped air holes were fabricated by Liu et al. [47]. Moreover, any types of complex structure can be fabricated using the extrusion technique [48, 49]. In addition, the manufacture of 3D printed dies using 3D printing technology paves the way for fabricating any types of asymmetrical air holes, including the elliptical shaped air hole structure [50]. Thus, using the existing fabrication technology, the proposed PCF sensor can be fabricated feasibly.

4. NUMERICAL RESULTS AND DISCUSSION

The intensity of light interaction with matter is shown in Fig. 2. It can be observed that light is well confined inside the core area. It can also be observed that the elliptical shaped air holes can cause an index difference between the x- and y-polarization modes because of their asymmetrical structure. The obtained effective refractive indices in the x polarization, 1 THz and \( W_c = 36 \mu m, 38 \mu m, \) and 40 \( \mu m \) are 1.326, 1.320, and 1.315, whereas for the y-polarization mode, the refractive indices are 1.344, 1.338, and 1.331, respectively. So, from the index difference, it is clear that higher-order modes can be present in the PCF. But when a light pulse is energized at the center of the core, only the fundamental modes will propagate through the core. For the other modes, the light will propagate through other regions except the core of the fiber [51]. So, our proposed fiber operates in the single-mode region.

The level of light interaction with ethanol at the core holes at different core air hole widths (\( W_c \)). 1 THz, and both x- and y-polarization modes is shown through Fig. 3 and Fig. 4, respectively. It can be observed that interaction of light intensity is better in the x-polarization mode than the y-polarization mode. Again, it can be observed that intensity of light increases with frequency starting from 0.4 THz, reaches a maximum position at 1 THz, and then starts to decrease.

The reason is that light confinement reaches an optimum position at 1 THz, and further increase of frequency causes the useful light to leak towards the cladding and also to the material. It can be seen that the maximum core power fraction is obtained at \( W_c = 40 \mu m \), and as \( W_c \) decreases, the amount of the core power fraction also decreases. The reason is that the amount of analyte filled inside the core holes decreases as \( W_c \) decreases, and hence the core power fraction also decreases.

Fig. 2. Mode field distribution for \( W_c \) of (a) 36 \( \mu m \), x-pol, (b) 36 \( \mu m \), y-pol, (c) 38 \( \mu m \), x-pol, (d) 38 \( \mu m \), y-pol, (e) 40 \( \mu m \), x-pol, and (f) 40 \( \mu m \), y-pol and at 1 THz frequency.

Fig. 3. Core power fraction versus frequency at different \( W_c \) and x-pol with \( f = 1 \) THz.

Fig. 4. Core power fraction versus frequency at different core air hole widths and y-pol with \( f = 1 \) THz.

Fig. 5. Relative sensitivity of ethanol with respect to frequency at different \( W_c \) and x-polarization mode.

Figures 5 and 6 illustrate the amount of relative sensitivity of ethanol with frequency at different \( W_c \) and orthogonal polarization modes. From the figures of sensitivity, it can be observed that sensitivity is better for x-polarization mode than the y-polarization mode. This is logical because the core power fraction in x-pol is better than y-pol. Therefore, we choose x-pol as optimum, as the main concern of our proposed terahertz PCF is sensing.
From Fig. 5, it can be observed that highest relative sensitivity is obtained at $W_c = 40 \, \mu m$ and 1 THz because the core power fraction is highest (Fig. 3) at that point. But, $W_c = 40 \, \mu m$ is the maximum width of air holes that can be fabricated without significant fabrication difficulties. Therefore, we choose $W_c = 38 \, \mu m$ as optimum because during standard fabrication, fluctuations of global parameters of a PCF may happen. Therefore, at optimum design conditions, the obtained relative sensitivity of ethanol is 68.8%. The obtained relative sensitivity in terahertz frequency range is better than the previously proposed sensors [10,11,13–16] operating in optical wavelength.

The characteristics of birefringence with respect to frequency at different $W_c$ is shown in Fig. 7. It can be observed that birefringence increases with the reduction of $W_c$. The reason is that the index difference between $x$- and $y$-polarization modes increases with core air hole width reduction. At optimum design parameters, the obtained birefringence is 0.0176 high ($>10^{-2}$), which is comparable to previously published [38,52,53,54] PCFs.

The characteristics of EML with respect to frequency at different core air hole widths are shown in Fig. 8. It is observed that EML decreases as core air hole width increases. This is true because increasing of core air hole width increases the amount of air inside the core, whereas the amount of material decreases, which consequently reduces the EML. It is also observed that EML increases with frequency, which is consistent with expectations, because according to the empirical equation of calculating material absorption loss [22], EML depends on frequency. The relation can be defined by the equation

$$a(\nu) = \nu^2 + 0.63\nu - 0.13 \, \text{[dB/cm]} \quad (11)$$

where $\nu$ is the normalized frequency. At optimum design parameters, the obtained EML is $\approx 0.05 \, \text{cm}^{-1}$, which is comparable to the previously proposed [38,52,53,54] optical waveguide.

The characteristics of EML with respect to frequency at different $W_c$ and $x$-polarization mode.

Fig. 6. Relative sensitivity of ethanol with respect to frequency at different $W_c$ and $y$-polarization mode.

Fig. 7. Birefringence versus frequency at different $W_c$.

Fig. 8. Effective material loss versus frequency at different $W_c$ and $x$-polarization mode.

Fig. 9. Confinement loss versus frequency at different $W_c$ and other optimum design conditions.

Fig. 10. Dispersion versus frequency at different core air hole widths with other optimum design conditions.
The property of confinement loss of the proposed PCF-based terahertz sensor is shown in Fig. 9. It can be seen that confinement loss decreases with the increase of frequency. This is because with the increase of frequency, the guided mode starts to confine strongly to the porous core region [32]. At optimum design parameters, the obtained confinement loss is 7.79 \times 10^{-12} \text{cm}^{-1}, which is negligible compared to the obtained EML. Also, the obtained confinement loss is comparable to the previously proposed [10,11,13–16] PCFs.

The property of dispersion of the proposed terahertz sensor with respect to frequency at different \( W_c \) is shown in Fig. 10. It can be observed that dispersion is flatter at \( W_c = 40 \mu \text{m} \) than \( W_c = 38 \mu \text{m} \) or \( W_c = 36 \mu \text{m} \), because as \( a = 40 \mu \text{m} \), the air holes get closer to each other, and thus the refractive index difference with frequency is lower. At optimum design parameters, the obtained dispersion variation is 1.08 ± 0.38 \text{ps/THz/cm} at a frequency range of 1–1.6 \text{THz} bandwidth, which is comparable to the previously proposed [22,23,28,38] optical waveguides.

The area covered by the intensities of light-matter interaction with respect to frequency is shown in Fig. 11. Figure 11 reflects that the effective area decreases when frequency increases. At optimum design parameters, the obtained effective area is 2 \times 10^5 \mu \text{m}^2, which is higher than the previously proposed [22,23,28,38].

The characteristics of NA with respect to frequency and different core air hole widths are shown in Fig. 12. It can be seen that NA decreases with the increase of frequency. A high value of NA is desirable for optical tomography application. At optimal design parameters, we obtain a NA of 0.37, which is comparable to the previously proposed optical sensor [37], whereas most of the previously proposed sensors [10–16] ignored mentioning this characteristic of PCF.

Throughout the whole characterization process of the proposed PCF-based terahertz sensor, we paid careful attention to the fabrication point of view. It is well known that ±2\% variation of fiber global structure may happen during the standard fabrication process of the fiber [55], so we considered ±2 \mu \text{m} variation of global parameters as optimum design parameters. Table 1 shows the characteristics comparison of the PCF-based sensor at optimal design parameters and ±2 \mu \text{m} variation of global parameters from the optimal.

5. CONCLUSION

A new type of PCF-based sensor is designed to operate in the terahertz frequency range. Using Zeonex as the background material, simulation results show a high relative sensitivity of 68.87\%, high birefringence of 0.0176, and negligible confinement loss of 7.79 \times 10^{-12} \text{cm}^{-1} at 1 \text{THz}. High relative sensitivity of ethanol is suitable for applications in the medical and food industries to detect the concentration of alcohol. Moreover, small dispersion variation, negligible confinement loss, and low EML are required for high data rate multichannel transmission application of terahertz waves. In addition, high birefringence and high NA are useful for polarization-preserving applications and filtering applications. The fabrication of the proposed terahertz sensor is readily possible using the existing fabrication technology. It is anticipated that this research work will open a new window to future research on terahertz sensors.

### Table 1. Comparison of the Proposed Terahertz Sensor at Optimal Design Parameters with ±2 \mu \text{m} Variation of Global Parameters

<table>
<thead>
<tr>
<th>Global Parameter Variation</th>
<th>Relative Sensitivity (%)</th>
<th>Core Power Fraction (%)</th>
<th>Birefringence (B)</th>
<th>( \alpha_{\text{eff}} ) (cm(^{-1}))</th>
<th>( \beta_2 ) (ps/THz/cm)</th>
<th>( L_c ) (cm(^{-1}))</th>
<th>NA</th>
</tr>
</thead>
<tbody>
<tr>
<td>+2 \mu m</td>
<td>71.94</td>
<td>69.128</td>
<td>0.019</td>
<td>0.045</td>
<td>1.09 ± 0.39</td>
<td>8.5 \times 10^{-12}</td>
<td>0.357</td>
</tr>
<tr>
<td>Optimum</td>
<td>68.87</td>
<td>67.05</td>
<td>0.0176</td>
<td>0.05</td>
<td>1.08 ± 0.38</td>
<td>7.79 \times 10^{-12}</td>
<td>0.356</td>
</tr>
<tr>
<td>-2 \mu m</td>
<td>65.34</td>
<td>63.7</td>
<td>0.0165</td>
<td>0.055</td>
<td>1.07 ± 0.37</td>
<td>6.12 \times 10^{-12}</td>
<td>0.355</td>
</tr>
</tbody>
</table>
REFERENCES