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A Highly Sensitive Photonic Crystal Fiber Gas Sensor for the Detection of Sulfur Dioxide

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Abstract

Sulfur dioxide (SO₂) is one of the most prevalent contaminants in the atmosphere. It is mostly generated as a byproduct of the burning of sulfur-containing coal and oils, as well as the smelting of various ores. SO₂ contributes to the development of major diseases such as asthma and chronic bronchitis. In this paper, we proposed a Wheel Structured circular air hole Photonic Crystal Fiber (WS-PCF) based gas sensor to detect SO₂ gas. The proposed WS-PCF gas sensor consists of a four-layer-thick circular cladding air hole. The diameter of the first layer varies throughout the optimization procedure, while the diameters of the succeeding three layers remain constant. The numerical investigation on the sensor parameters such as numerical aperture, effective area, non-linearity, confinement, loss and the relative sensitivity of the proposed sensor are extensively analyzed in a wavelength range of 0.9 µm to 1.2 µm. The proposed WS-PCF gas sensor offers the highest relative sensitivity of 83.64% and a lower confinement loss of $6.34 \times 10^{-9} dB/km$. The proposed sensor is simple and offers 14% high sensitivity and very low confinement loss (10^{-3} reported in literature) compared with the exist literature.

Keywords WS-PCF gas sensor \cdot Circular cladding \cdot Relative sensitivity \cdot Confinement loss \cdot Non-linearity and numerical aperture

1 Introduction

Technical advancements in detecting gas concentration and composition, such as Volatile Organic Compounds (VOC), are urgently needed for the early detection of gas leaks and explosions as industrial automation and artificial intelligence increase [1–3]. Gas sensors use electro-chemistry, contact combustion, optical spectroscopy, chemical absorption, and other mechanisms to work [4–6]. Optical signals travel through the optical fiber and respond to the environment in the detection zone, which is made up of different fiber configurations. The optical fiber's characteristics make it a

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suitable candidate for constructing high-performance gas sensors in recent years [7–9]. The interference and resonance enhancement in various unique fiber topologies significantly enhanced the optical fiber gas sensor's sensitivity [10, 11].

Due to its high sensitivity, small size, and flexibility, the PCF-based sensor is precious. The characteristics can be determined by optimizing the size, shape, and position of the core and cladding, as well as by varying the pitch calibration. In PCF sensors excellent optical properties are achieved due to the distribution of holes. Moreover, there is a scope of tuning the optical property of the PCF sensor by altering the arrangement, size and shape of the holes. These parameters are difficult to achieve with conventional optical fiber [12–14].

PCF is resistant to the external environment, it measures minute temperature variations quickly, and it can also detect various gases and chemicals that are harmful to humans. Different sensors are used for the detection of different parameters. The PCF based SPR sensor concurrently measures RI, magnetic field and temperature [15] and SPR sensor which detects liver tissue [16]. The PCF is used in a variety of sensing applications, including temperature, bio-sensing, gas sensing, and temperature sensing [17–25]. The presence of

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air holes in a PCF cladding enables both direct light transmission and the introduction of analytes (gases, chemicals, etc.) into the air holes, resulting in constrained light interaction with the sample and the development of novel sensing applications [26].

The main objective of this paper is to demonstrate the detection of SO_2 at a temperature of 25 °C. SO_2 is a colorless, flammable, reactive gas with a pungent odour. It is produced in a variety of natural and human-made ways. SO_2 emissions are primarily caused by the combustion of high-sulfur coal and heating oil in power plants, followed by industrial boilers and metal smelting [27]. When asthmatic children and adults exercise outdoors, SO_2 can temporarily impair breathing. Short-term exposure of asthmatic individuals to elevated SO_2 levels while moderately exercising may result in diminished lung function, which may manifest as wheezing, chest tightness, or shortness of breath [28].

In this paper a high sensitivity WS-PCF sensor is proposed for SO₂ gas detection compared with existing methods. To sense the SO₂ gas, light confinement occurs in the area of the core at wavelengths ranging from 0.9 μ m to 1.3 μ m. The performance of the WS-PCF gas sensor is simulated by COMSOL Multiphysics software and analysis are carried for different sensing parameters. The sequence of the manuscript is as follows: sensor design, numerical analysis, results and discussion, and conclusion.

2 Proposed Gas Sensor Design

Figure 1 illustrates the cross-section view of the proposed WS-PCF gas sensor. The design incorporates a circular core surrounded by four layers of cladding. The diameter of the third, fifth, ninth, and eleventh air holes in the first cladding layer is $1.26 \mu m$. The cladding has 12 air holes in each of the four layers. The diameter of second cladding layer is 0.635 μm . The diameter of third and fourth cladding layers

has a diameter of 0.705 μ m. The core is located in the centre, where light confinement occurs, and measures 1.27 μ m in diameter. The WS-PCF gas sensor's sensing capability is determined by several critical parameters, one of which is the pitch. Pitch is the distance between center to center air hole and is represented as Λ . The design maintains a 2 μ m pitch. The performance of the gas sensor is investigated by varying the diameter of the 3rd, 5th, 9th, and 11th cladding air holes. Silica is used as a background material because it is more efficient than other materials due to its 1.45 Refractive Index (RI). The core is filled with SO₂ gas having a RI of 1.3396, while the cladding is filled with air having a RI of 1. The Perfectly Matched Layer (PML) that surrounds the gas sensor design prevents light from scattering. The proposed WS-PCF gas sensor has a PML of 0.8 μ m.

The gas is sensed in the hollow core of the PCF gas sensor. The RI of the gas to be sensed is placed in the core, where light and the gas samples overlaps with each other. When the gas is passed to the core of the hollow core of the PCF gas sensor there is a deviation at the output of the sensor and it is measured by Beer-Lambert law. The deviated output gives the sensitivity of the gas to be sensed.

Various factors are studied, including sensitivity, confinement loss, effective refractive index (n_{eff}) , effective mode area (A_{eff}) , non-linearity, and numerical aperture (NA). Due to the difficulty associated with fabrication, the proposed WS-PCF gas sensor's core and cladding are circular. Numerous fabrication methods are available. Among the most prevalent are drilling, die-casting, stack and draw, and sol-gel fabrication. However, only a few of these fabrication procedures offer exceptional outcomes. Stack and draw will produce superior results during the circular air hole construction process. However, the disadvantage of this process is that if the design is intricate, the final production may deviate from the original. To address this issue, a sol-gel manufacturing process is used to construct this WS-PCF gas sensor efficiently.



of 0.8 µm to 1.3 µm Sensitivity (%)

Table 1 Sensitivity for different cladding diameter for the wavelength

Sensitivity (70)						
λ (μm)	1.26 µm	1.27 µm	1.28 µm	1.29 µm		
0.8	83.733	63.497	35.427	66.81		
0.9	23.799	25.829	31.656	34.195		
1	51.785	45.538	43.809	41.635		
1.1	62.65	62.785	62.992	62.496		
1.2	82.676	83.057	83.377	83.646		
1.3	66.553	76.333	81.045	82.791		

3 Mathematical Equations

Due to the limited number of air holes, optical power radiates from the core and leaks into the cladding region, resulting in confinement loss. The wavelength and imaginary part of the n_{eff} affect confinement loss, which can be calculated as [29]

$$L_c = 8.686k_0 x I_m (n_{eff}) x 10^6 \tag{1}$$

$$k_0 = \frac{2\pi}{\lambda}$$

where L_c is the confinement loss, k_0 is the free space wave number, and $I_m(n_{eff})$ is the N_{eff}'s imaginary part. Beer-Lambert law is used to calculate the deviation in light intensity, as light and gas elements interrelate in the core. The mathematical formula is given as [30]

$$I(\lambda) = I_0(\lambda) \exp(-r\theta_m LC) Wm^{-2}$$
⁽²⁾

where $I(\lambda)$ and $I_0(\lambda)$ Represent the amplitudes of light signal with and without gas samples, respectively. r is the relative sensitivity, θ_m is the absorption coefficient, L is the fiber length, C is the gas concentration, and λ is the SO₂ absorption wavelength.

The phenomenon of shared action between the gas components and guiding light at an exact wavelength is relative sensitivity. The Beer-Lambert law states that relative sensitivity varies with gas attention and wavelength, which can be calculated as [31]

$$r = \frac{n_r}{n_{eff}} X f \tag{3}$$

where n_r denotes SO₂'s RI, n_{eff} denotes SO₂'s modal effective RI, and f denotes frequency of relative sensitivity. Furthermore, the coefficient is defined as the ratio of optical power in core to the total power of device, which is calculated as [32]

$$f = \frac{\int_{\text{Sample}} \text{Re}(\text{E}_{x}\text{H}_{y} - \text{E}_{y}\text{H}_{x})\text{dxdy}}{\int_{\text{total}} \text{Re}(\text{E}_{x}\text{H}_{y} - \text{E}_{y}\text{H}_{x})\text{dxdy}} \times 100$$
(4)

 E_x and E_y are the electric fields of x and y elements, and H_x and H_v are the magnetic fields of x and y fundamentals.

During optical power propagation through the core, light concentrates on a precise area that differs from the geometrical size of the core and this area is known as the A_{eff}. It can be calculated using Eq. (5) given in [33]

$$A_{eff} = \frac{(\iint |E|^2 dx dy)^2}{\iint |E|^2 dx dy} \mu m^2$$
(5)

where A_{eff} is the effective area of the core and E denotes the guided mode's transverse electric fields. Other parameters considered for the fiber optic gas sensor design is nonlinearity. The higher nonlinearity-based PCF value is used for signal processing. Non-linearity is inversely proportional



Fig. 2 (a) the confinement loss versus wavelength for various core diameters, (b) Relationship between confinement loss and cladding diameter



Fig. 3 (a) Variation in relative sensitivity as a function of air hole diameter in the cladding. (b) Enlarged view of sensitivity graph and (c). The relative sensitivity vs the cladding air hole diameter at $1.2 \,\mu m$ wavelength

to the A_{eff} of the core, which can be calculated using the equation [34].

$$Y(\lambda) = \frac{2\pi * n_2}{\lambda * A_{eff}} \mathbf{W}^{-1} m^{-1}$$
(6)

The non-linear co-efficient of silica material is represented as n_2 .

The light gathering capacity of the fiber is calculated by Numerical Aperture (NA), as given by the following equation.

$$NA = \frac{1}{\sqrt{1 + \frac{\pi x A_{\text{eff}}}{\lambda^2}}}$$
(7)

The concentration of the SO_2 gas can find by using the following formula

$$n = 1 + \frac{\alpha x \rho}{2} \tag{8}$$

where, α is molecule palarizability and its value is 3.882. ρ is number of molecules per unit volume.

4 Numerical Analysis and Discussions

To detect SO₂, a WS-PCF gas sensor is used, and the diameter of the cladding air holes is varied. The diameters of the third, fifth, ninth, and eleventh air holes in the first cladding layer are analyzed. The values of different diameters are 1.26 μ m, 1.27 μ m, 1.28 μ m, and 1.29 μ m. Sensing parameters like sensitivity, A_{eff}, confinement loss, non-linearity and numerical aperture are analyzed for different cladding diameters of 1.26 μ m, 1.27 μ m, 1.28 μ m, and 1.29 μ m. For





the purpose of optimize the wavelength values from 0.8 μm to 1.3 μm are analyzed and it is tabulated in Table 1.

From Table 1 the sensitivity for all the four different cladding diameters are linearly increasing for the wavelength

between 0.9 μ m and 1.2 μ m. Above and below these wavelength ranges the sensitivity is not linear. As the size of the first cladding layer increases, the sensitivity increases. At 1.29 μ m of the first layer cladding layer diameter the



Fig. 5 (a) Non-linearity variation with respect to wavelength and (b) Graph between non-linearity vs different cladding diameter at 1.2 µm wavelength



Fig. 6 (a) NA vs wavelength for different first layer cladding diameter and (b) Graph between NA and different cladding diameter at $1.2 \ \mu m$ wavelength

best sensitivity of 83.64% is achieved for the wavelength of $1.2 \,\mu\text{m}$.

The confinement loss or loss curve is explained through Eq. (1). Figure 2(a) illustrates the loss curves for various cladding diameters in relation to wavelength, while Fig. 2(b) illustrates the loss curves in relation to cladding diameter for wavelengths ranging from 0.9 μ m to 1.2 μ m. The core area's light confinement is superior because the confinement loss is less as the wavelength propagates. In comparison, as the diameter of the cladding in the first layer increases, the confinement loss increases from 4.32×10^{-8} to 6.34×10^{-9} dB/km. This increase in confinement loss will have no effect on the PCF gas sensor's performance.

The proposed WS-PCF gas sensor is demonstrated in the gas sensing application. The sensible response depends mainly on the wavelength because the light-mater interaction is not the same for all-optical wavelengths. In Fig. 3(a), for different first layer cladding values of 1.26 µm, 1.27 µm, 1.28 µm, and 1.29 µm the sensitivity is plotted against the wavelength. The sensitivity is increased as wavelength increases. It means higher the optical wavelength and stronger the light-mater interaction. Figure 3(b) is the enlarged view of the sensitivity graph. In Fig. 3(c), the graph is drawn for the sensitivity w.r.t different cladding diameter. It is clearly shown that as the size of the cladding diameter increases, the sensitivity of WS-PCF gas sensor is increased due to more light is confined in the core region. The sensitivity of 1.29 µm cladding diameter compares high in the other three cladding diameters. The sensitivity of 1.26 µm cladding diameter is 82.676%, and the large cladding area of 1.29 μ m is 83.646%.

Light confinement in a particular core area for a specific wavelength is called as A_{eff} . The A_{eff} increases linearly with wavelength for all cladding diameters this is due to the leakage of modes through the air holes. The graphs in Figs. 4(a) and 4(b) illustrate the A_{eff} in relation to the wavelength and the enlarged A_{eff} , respectively. It is understood that as the diameter of the cladding increases, the A_{eff} decreases, as illustrated in Fig. 4(c). A low A_{eff} of 0.155 μ m² is achieved for first layer cladding diameter of 1.29 μ m.

Non-linearity is a critical parameter in signal processing; a small effective area indicates a high power density is required for non-linear effects to be significant [35]. For optimal signal processing, the nonlinearity should be high. The nonlinearity for various cladding diameters is illustrated in Fig. 5(a). It is discovered that non-linearity decreases with increasing wavelength. Figure 5(b) Illustrates the non-linearity graph for various cladding diameters; as the cladding diameter increases, the non-linearity increases because the nonlinearity and A_{eff} are inversely proportional to each other. As a result, the proposed WS-PCF gas sensor is an attractive candidate for nonlinearity. It is concluded that signal processing in this PCF gas sensor is more efficient at large cladding diameters.

The NA graphs for various cladding areas are shown in Figs. 6 (a) and 6 (b). The NA decreases slightly with increasing frequency due to an increase in the difference in effective mode indices between cladding and core.



Fig. 7 (a) Cladding diameter dependence of non-linearity and A_{eff} for proposed WS-PCF gas sensor, (b) Cladding diameter dependence of sensitivity and A_{eff} and (c) Cladding diameter dependence of N.A and A_{eff}

From the Fig. 6, it is inferred as the size of the cladding diameter increases then there is a small increase in the numerical aperture at 1.2 μ m wavelength this is due to the property of the N.A, were the light observing capacity is increased as the size of the cladding increased, The A_{eff} is a quantitative measure of the transverse area that covers a waveguide or fiber mode. The sensitivity, non-linearity, and numerical aperture for four different first layer cladding diameters of 1.26 μ m, 1.27 μ m, 1.28 μ m, and 1.29 μ m are compared with the A_{eff}. The four different cladding areas are 1.26 μ m, 1.27 μ m, 1.28 μ m, and 1.29 μ m; it is shown in Fig. 7. Further, the analysis is carried out to verify the relationship between non-linearity, mode area, sensitivity and N.A for different cladding diameter. Figure 7(a) Illustrates, the effect of the diameter of the air hole in the first layer cladding on the mode area and relative sensitivity. Increases in the diameter of the first cladding air holes result in an increase in light confinement in the core region, this is due to more light is confine in the core region. As a result of the strong interaction between light and gas passing through the air hole, the A_{eff} through the core region is reduced, while the relative sensitivity of the SO₂ gas sensor is increased. Due to the inverse relationship between nonlinearity and A_{eff} , nonlinearity increases as cladding diameter increases, while mode area decreases in relation to cladding diameter, as illustrated in Fig. 7(b). As illustrated in Fig. 7(c), as the diameter of the cladding increases, the A_{eff} decreases, allowing for an increase in light

Table 2	Different concentrations	of	SO_2	gas
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S.No	Concentration of SO ₂ gas (PPM)	Refractive index	Sensitivity (%)
1	174,600	1.3388	81.919
2	174,700	1.3390	82.379
3	174,800	1.3392	82.824
4	174,900	1.3394	83.248
5	175,000	1.3396	83.646
6	175,100	1.3398	84.018
7	175,200	1.3400	84.363
8	175,300	1.3402	84.681
9	175,400	1.3404	84.974
10	175,500	1.3406	85.244

From the Table 2 it is understood that, as the concentration of SO₂ gas is increased, the RI and sensitivity of WS-PCF gas sensor is increases. Based on the concentration of the SO₂ gas the sensitivity varies, it means that the concentration of SO₂ and sensitivity are mutually proportional to each other (Fig. 8).

Table 3 compares the WS-PCF gas sensor to various structures for sensing different gases. The proposed WS-PCF gas sensor gives the best sensitivity and confinement loss of 83.646% and 6.34×10^{-09} dB/km respectively at 1.2 μ m wavelength. By adjusting the diameter of the first layer cladding air hole, a maximum sensitivity of 83.646% is obtained, which is extremely high for the detection of SO₂ gas in comparison with V-PCF, H-PCF and micro-cored photonic PCF sensor [40, 41].

Table 3Comparison of the proposed WS-PCF gas sensor	S.No	PCF Sensor	Sensitivity (%)	Confinement loss
with other PCF sensors 1		HPC-PCF [36]	21.2	0.000025 dB/m
2	2	C-PCF [37]	72.04	
3	;	Q-PCF [38]	64.69	$4.38 \times 10^{-06} \text{ dB/km}$
4	Ļ	Triangular-PCF [39]	75.14	$1.41 \times 10^{-02} \text{ dB/m}$
5	i	H-PCF for sensing SO ₂ [40] V-PCF for sensing SO ₂ [40]	58.34 59.34	$8.94 \times 10^{-04} \text{ dB/m}$ $5.93 \times 10^{-04} \text{ dB/m}$
6	5	Micro-cored photonic crystal fiber for sensing SO ₂ [41]	70	0.000136525 dB/m
7	,	Microstructure based gas sensor for ammonia detection [42]	70.25	$1.202 \times 10^{-1} \text{ dB/m}$
8	8	Proposed WS-PCF at 1.29 μ m for sensing SO ₂	83.646	$6.34 \times 10^{-09} \text{ dB/km}$

gathering capacity; as light gathering capacity increases, the NA increases as well. These analyses indicate that the WS-PCF sensor as designed is well suited for gas sensing applications. The RI and sensitivity of SO2 gas is calculated using the Eq. (8) and the corresponding values are tabulated in Table 2.



Fig. 8 Sensitivity depends on RI and concentration of SO₂ gas

5 Conclusion

This paper aims to improve the relative sensitivity of the proposed sensor for sensing SO₂ gas while reducing the fabrication complexity. It investigates the performance of the proposed WS-PCF gas sensor by increasing first layer cladding diameter. The different cladding diameters are 1.26 µm, 1.27 µm, 1.28 µm, and 1.29 µm. High sensitivity and confinement, loss of 83.646% and 6.34×10^{-09} dB/km respectively, is achieved for 1.29 µm diameter, and it is best compared with the previous methods. The combustion of fossil fuels transports SO₂, and it is a naturally occurring byproduct of volcanic eruptions. SO2 causes severe issues to the human, especially in the respiratory tract. The proposed structure is easy to fabricate due to its simple design. The proposed WS-PCF gas sensor can detect colorless gas, and it is used as a biosensor.

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Data Availability Data and materials are associated with the manuscript.

Declarations

Ethics Approval Yes.

Consent to Participate All the authors in this investigation voluntarily agree to participate in this research study.

Consent for Publication All authors provide consent for publication.

Competing Interests There are no competing interests.

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