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RESEARCH ARTICLE

Chemical sensing through photonic crystal fiber: sulfuric acid detection

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Abstract A photonic crystal fiber (PCF) for sensing of sulfuric acid is designed and analyzed using Comsol Multiphysics. To analyze the sensor performance, 0%, 10%, 20%, 30%, 40% H_2SO_4 solution is placed into the fiber separately and then relative sensitivity, confinement loss, birefringence, effective area etc. are investigated for each solution over wavelength ranging from 0.8 to 1.8 μm. The sensor structure affords moderately high relative sensitivity and around 63.4% sensitivity is achieved for the highest concentration of H_2SO_4 at the wavelength 1.5 μm in x polarization direction. This PCF model also shows zero confinement loss for all solutions of H_2SO_4 over wavelength ranging from 1 to 1.35 μm and later on approximately 1.422×10^{-17} dB/km confinement loss is found for the highest concentration of H_2SO_4 at 1.5 μm wavelength. Besides, higher birefringence is attained when the concentration of sulfuric acid is lower and it is achieved 7.5×10^{-4} at 1.5 μm wavelength. Moreover, higher sensing area is achieved at high concentration of sulfuric acid.

Keywords refractive index, confinement loss, birefringence, relative sensitivity

1 Introduction

Sulfuric acid is an essential industrial substance. It is extensively used for almost every manufacturing purposes. Fertilizers making is the prime usage of it and it is also useful in manufacturing of chemicals like hydrochloric acid, nitric acid, sulfate salts, synthetic detergents, and drugs. It serves as battery acid where 33% H_2SO_4 is used. The amount of sulfuric acids' concentration in any product needs to be precious. So, precise detection of sulfuric acid is very demanding. The development of optical fiber technology has enlarged the telecommunication [1,2] and chemical sensing field [3,4]. The smart version of optical fiber is photonics crystal fiber (PCF) and it provides with some extraordinary characteristics for example light propagation through the fiber with zero dispersion [5], low confinement loss [6], high nonlinearity [7,8] etc. Recently, sensing of liquid and chemical through optical fiber has made huge interest among researchers where PCF is the latest version of conventional optical fiber. To enlarge chemical sensing performance through PCF, already noteworthy labors have been given by researcher [9,10]. Sensing properties of PCF based chemical sensor can be adjusted by varying size and position of air holes in both core and cladding region as well as chemical concentration [11,12]. Sensitivity and confinement loss are regarded as the two main guiding properties for liquid and chemical sensing applications. Birefringence is said to be one of the most splendid optical properties of PCF. A high value of birefringence is always desired which can be achieved by either terminating the symmetry of the fiber cladding or initiating asymmetry to the fiber core [13]. The polarization state in cylindrical optical fiber operates in a few meters. PCFs having a high value of birefringence are highly recommended for numerous applications like long-distance communications, sensing purposes, polarization-sensitive optical modulators, etc. [14,15]. Numerous research works are currently running in order to achieve a maximum sensitivity and confinement loss at a minimum state at the same time [16]. In recent times, several types of geometric structures have been proposed by the researchers for the betterment of relative sensitivity and degradation of confinement loss at a satisfactory level. A micro-

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structured PCF model where sore-cladding regions were reconstructed with circular air holes for aqua sensor is proposed by Adamgil [17], which results in a relative sensing coefficient of 9% and a low confinement loss in the order of 10^{-1} dB/m for ethanol. After that in 2015, Adamgil and Haxha have presented PCF model for liquid sensing applications with high sensitivity as well as high birefringence. That time they got around 24% relative sensitivity and 2.40×10^{-4} birefringence [18]. Again in 2016, they reported a PCF structure for sensing analytes in aqueous solutions where birefringence as well as relative sensitivity became higher than before [19]. A hybrid PCF (H-PCF) model which was organized by elliptical and circular individual air holes was suggested by Asaduzzaman et al. [20]. Their simulated result brought out high sensitivity (about 48% for ethanol at 1.55 μm wavelength) and low confinement loss for benzene, ethanol and water than the prior PCFs because their proposed PCFs are made with three rings that can be used for sensing applications of industrially valuable lower indexed chemicals. From the above discussion we can conclude that, the sensitivity level entirely depends on air holes management and the numbers of layers in the cladding area. Although very few numbers of PCF based liquid sensors were presented [21–23], but they are still in proposed condition. For this reason, there are still chances for development of PCF-based liquid sensing. The fundamental objective of this research is to design and analysis PCF sensor for sulfuric acid sensing. To observe the sensor performance, power confinement, relative sensitivity, confinement loss and birefringence are analyzed.

2 Model design

We have designed a PCF sensor structure where cladding region is made of 3 air hole layers and the radius of each circular air hole is 0.975 μm. Total fiber radius is 11.27 μm where a perfectly matched layer (PML) is taken as a boundary condition of 1 μm. In the core region, 6 outer elliptical holes are taken with *a*-semiaxis of 0.5333 μm, and *b*-semiaxis of 1.067 μm and they are placed 3.45 μm far from the center point of the fiber. Again, 4 middle elliptical holes are taken with *a*-semiaxis of 0.356 μm, and *b*-semiaxis of 0.64 μm and they are placed 1.0952 and 1.5333 μm far from the center point of fiber in positive and negative *x* and *y* direction respectively. Another 4 middle circular holes are taken with radius having 0.5333 μm and they are placed around 1.484 μm from the center point of fiber in positive and negative *y* direction. Moreover, a large elliptical central hole is also taken with *a*-semiaxis of 2.4 μm, and *b*-semiaxis of 0.8 μm. The proposed PCF sensor model and its light propagation direction through the analyte are shown in Figs. 1 and 2, respectively.

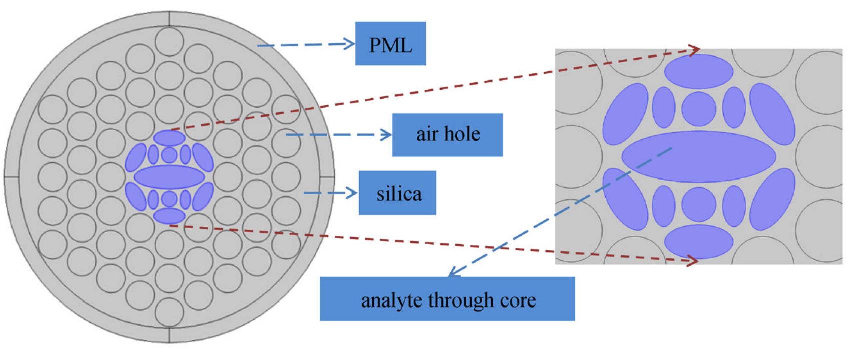

Fig. 1 Cross-sectional view of proposed PCF geometry

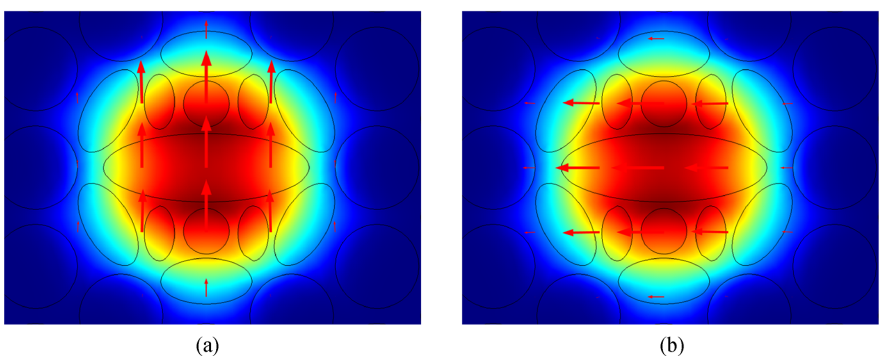

Fig. 2 Schematic presentation of (a) light propagation in *y* polarized direction, and (b) light propagation in *x* polarized direction

In left side of Fig. 1, the fiber material (silica), air hole and PML layer are marked and in the right sight zoomed blue color core region is displayed. In the core, we used different concentrations of sulfuric acid as analyte. Again, Fig. 2(a) represents traveling of light in y polarized direction where Fig. 2(b) shows light propagation in x polarized direction.

If we think about of the presented PCF sensor model fabrication, then yes, it is possible to fabricate this presented PCF sensor structure. Nowadays, many fiber fabrication methods have been employed for instance stacking, drilling, 3D printing, etc. Stacking method is useful to fabricate circular holes, where the 3D printing is useful to fabricate asymmetric (elliptical and rectangular holes) PCF structure. Very recently, Max Plank Institute has already fabricated few asymmetric shapes like elliptical, rectangular, etc. [24].

3 Method and analysis

The refractive index of any material defines the speed of light through that material. So the speed of light in any material varies with the refractive index of that material. It also changes according to the corresponding wavelength for both fiber material as well as liquid material where the refractive index of air hole is assumed to be unchanged (n_a = 1). Table 1 shows the change in refractive index against the variation of wavelength.

Table 1 Wavelength versus refractive index [25]

wavelength/μm	refractive index of silica
0.8	1.452
0.9	1.451
1.0	1.45
1.1	1.449
1.2	1.448
1.3	1.447
1.4	1.446
1.5	1.445
1.6	1.443
1.7	1.441
1.8	1.439

The refractive index of sulfuric acid also changes with respect to its concentration. When its concentration amount be large then refractive index also increases. In COMSOL Multiphysics, we have considered different concentration of sulfuric acid by putting the value of refractive index corresponding to specific concentration of sulfuric acid. Table 2 shows the change in refractive index against sulfuric acids' concentration at wavelength ranging from 0.8 to 1.8 μm.

Table 2 Sulfuric acids' concentration versus refractive index [26,27]

wavelength /μm	refractive index of H_2SO_4				
	0% H_2SO_4	10% H_2SO_4	20% H_2SO_4	30% H_2SO_4	40% H_2SO_4
0.8	1.329	1.3451	1.3576	1.3701	1.3821
0.9	1.328	1.344	1.3565	1.369	1.381
1.0	1.327	1.343	1.3555	1.368	1.38
1.1	1.326	1.342	1.3545	1.367	1.379
1.2	1.3245	1.3405	1.353	1.3655	1.3775
1.3	1.323	1.339	1.3515	1.364	1.376
1.4	1.321	1.337	1.3495	1.362	1.374
1.5	1.319	1.335	1.3475	1.36	1.372
1.6	1.317	1.333	1.3455	1.358	1.37
1.7	1.3145	1.3305	1.343	1.3555	1.3675
1.8	1.312	1.328	1.3405	1.353	1.365

In COMSOL Multiphysics, we designed a simple PCF structure where cladding region is in hexagonal shape and core region is made of 11 elliptical holes and 2 circular holes. Sulfuric acid is inserted through the core area and user controlled mesh is taken to select the specific area where we want to propagate the laser light. Parametric sweep is used to run the simulation for wavelength ranging from 0.8 to 1.8 μm.

Refractive index of any material is the measure of variation in light speed when it passes from vacuum to any material. It is expressed by

$$n = \frac{c}{v}. \tag{1}$$

Here, c is the speed of light in vacuum and v is the velocity of light in any medium.

In regular fiber, due to some imperfections the refractive indices for the principal axes x and y are different. To enrich the figure of merit in polarization-mode dispersion

(PMD) compensation, large differential group delay or equivalently high birefringence, is required along with a low propagation loss. Birefringence can be calculated by [28,29]

$$B_f = |n_y - n_x|. \quad (2)$$

Here, n_x is the refractive index in x polarization direction and n_y is the refractive index in y polarization direction.

The relative sensitivity is investigated by using Eq. (3) [30,31].

$$r = \frac{n_r}{n_{eff}}. \quad (3)$$

Here, n_r is refractive index of sensing liquid and n_{eff} is effective mode index.

Again, f is the power ratio which can be obtained by Eq. (4) [30,31].

$$f = \frac{\int_{\text{analyte}} R_e(E_x H_y - H_x E_y)\mathrm{d}x\mathrm{d}y}{\int_{\text{all}} R_e(E_x H_y - H_x E_y)\mathrm{d}x\mathrm{d}y} \times 100. \quad (4)$$

Here, E_x, E_y and H_x, H_y are the transverse electric field and magnetic field, respectively.

Sometimes, the arrangement of core-cladding of PCF causes a decrease in optical confinement that is called the confinement loss, L_c and it is given by [31–33]

$$L_c = 8.686 K_0 I_m[n_{eff} \times 10^3], \quad (5)$$

where, $K_0 = 2\pi/\lambda$, λ is the wavelength, and $I_m[n_{eff}]$ is imaginary part of effective mode index.

Always, light does not propagate to the whole core area where we put the analyte. To know the effective sensing area, we need to investigate the effective area which depends on electric field (E) and it can be calculated by [6]

$$A_{eff} = \frac{\left(\iint |E^2| \mathrm{d}x\mathrm{d}y\right)^2}{\iint |E^4| \mathrm{d}x\mathrm{d}y}. \quad (6)$$

4 Simulation results

After passing light through different concentration of sulfuric acid (sensing liquid), we got the effective refractive index in both x and y polarized directions from COMSOL Multiphysics and then using MATLAB, we plotted all output curves. Figures 3 and 4 show the effective refractive index in y and x polarization mode respectively for wavelength ranging from 0.8 to 1.8 μm.

From Figs. 3 and 4, it is evident that effective refractive index decreases with increasing wavelength in both polarized directions and it is logical because with increasing wavelength for a specific frequency the light speed in any medium increases, for this reason effective refractive index decreases as light speed in vacuum is constant. From the COMSOL Multiphysics simulation we can observe the effective refractive index in both polarized directions by selecting arrow surface mode and we got higher effective refractive index in y polarized direction than x polarized direction.

To use PCF sensor in polarization maintaining application, PCF sensor should have high birefringence. Figure 5 shows the birefringence profile for the proposed PCF model which is basically the difference effective refractive index between y and x polarized directions.

Figure 5 represents that birefringence is increasing with the increasing of wavelength. Again for larger

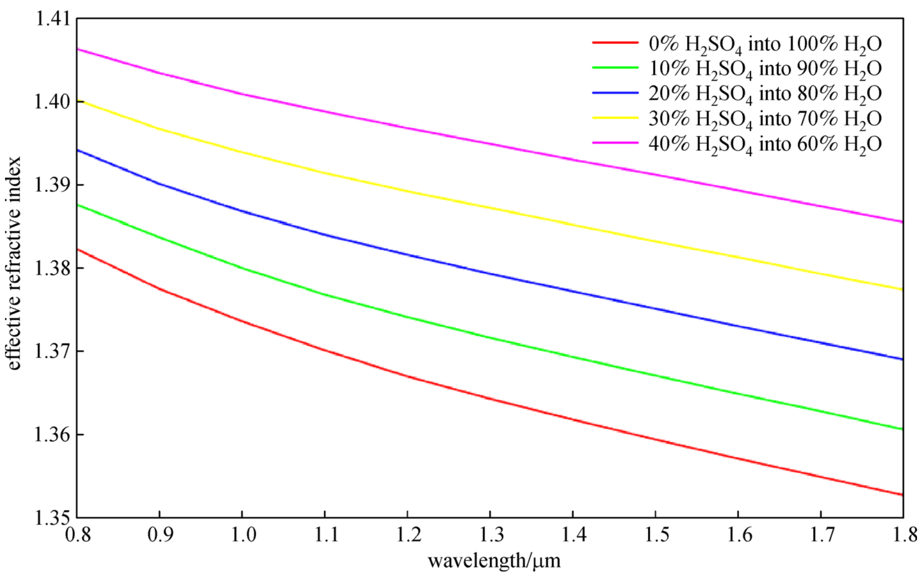

Fig. 3 Effective refractive index in y polarized direction for different sulfuric acid concentrations

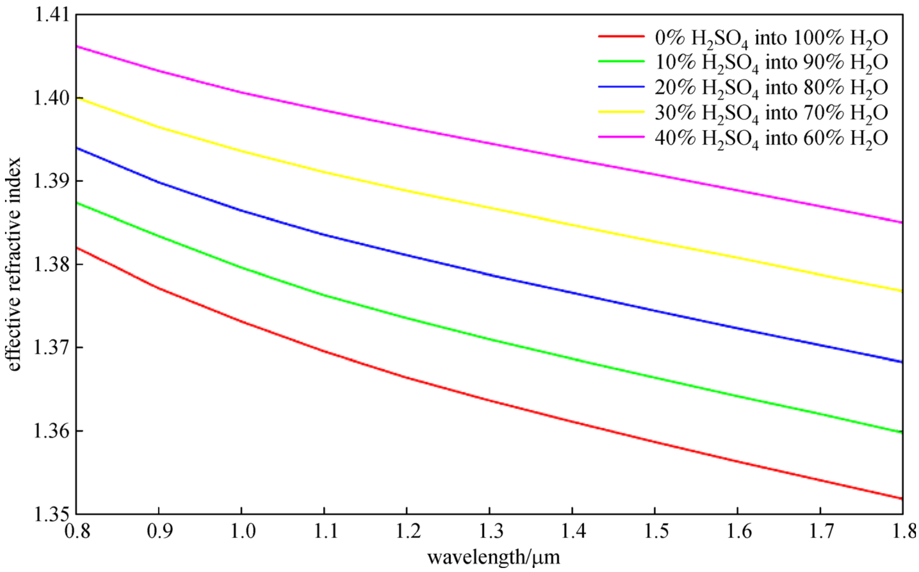

Fig. 4 Effective refractive index in x polarized direction for different sulfuric acid concentrations

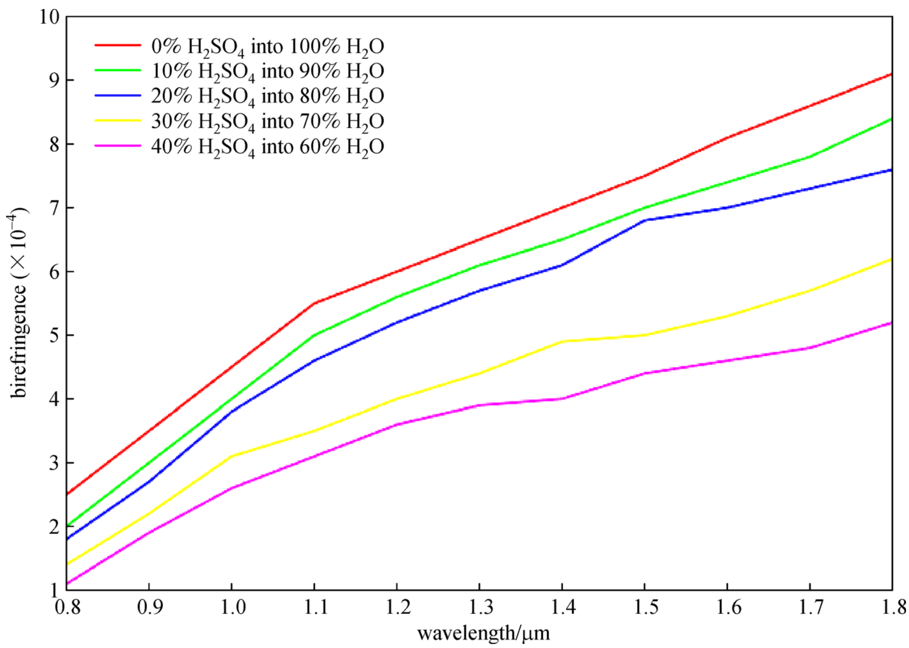

Fig. 5 Birefringence vs. wavelength for different sulfuric acid concentrations

concentration of sulfuric acid the birefringence seems declining, and the reason is that, with increasing sulfuric concentration the refractive index difference between core material and fiber material is decreasing in both x and y polarized directions. For this reason, effective refractive index difference between both directions decreases with increasing sulfuric acids' concentration. The PCF structure provides around 0.00075, 0.0007, 0.00068, 0.0005, 0.00044 birefringence at wavelength 1.5 μm for 0%, 10%, 20%, 30%, 40% H_2SO_4 solution respectively.

We got power ratio directly from COMSOL Multiphysics simulation and Table 3 shows the power ratio with respect to sulfuric acid concentration for wavelength ranging from 0.8 to 1.8 μm.

According to Table 3, power ratio is increasing with the increase of wavelength and it is logical as with increasing wavelength the light confinement through sulfuric acid area is increasing. Again with increasing sulfuric acid concentration the power ratio is also increasing. It happens because with increasing sulfuric acid concentration overall refractive index in core region increases and for this reasons more light confine through the core area is

Table 3 Sulfuric acids' concentration vs. power ratio

wavelength/μm	power ratio				
	0% H_2SO_4	10% H_2SO_4	20% H_2SO_4	30% H_2SO_4	40% H_2SO_4
0.8	46.9	50.67	52.888	55.232	57.132
0.9	52.01	53.285	56.043	57.683	59.199
1.0	55.04	56.566	57.971	59.313	60.572
1.1	56.911	58.108	59.284	60.422	61.497
1.2	58.15	59.173	60.187	61.176	62.113
1.3	59.008	59.905	60.801	61.677	62.508
1.4	59.592	60.396	61.202	61.99	62.737
1.5	59.972	60.705	61.439	62.158	62.839
1.6	60.193	60.87	61.549	62.212	62.839
1.7	60.288	60.922	61.556	62.175	62.759
1.8	60.281	60.88	61.479	62.062	62.611

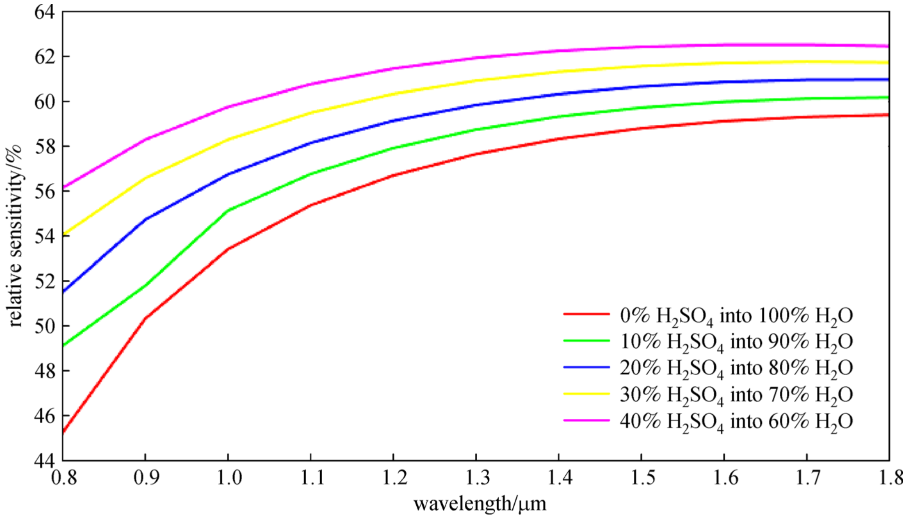

Fig. 6 Relative sensitivity in *y* polarization direction for different sulfuric acid concentrations

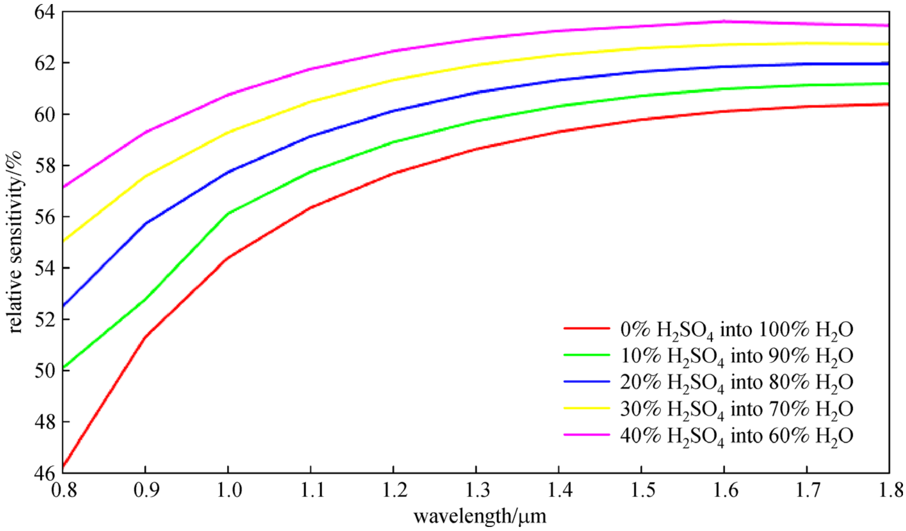

Fig. 7 Relative sensitivity in *x* polarization direction for different sulfuric acid concentrations

observed.

Figures 6 and 7 show the relative sensitivity curve which is calculated by using Eqs. (3) and (4) and it depends on power ratio, sulfuric acids' refractive index in different concentration and effective refractive index. From Figs. 6 and 7, it is evident that sensitivity is increasing with increasing wavelength for both polarized directions. It is meaningful as with increasing wavelength the light confinement through sulfuric acid area is increasing. Also, with increasing sulfuric acids' concentration the relative sensitivity is also in an increasing trend. It is also logical because with increasing sulfuric acid concentration overall refractive index in core region increases, and for this reason more light confine through the core area is observed. Again if someone thinks about the relative sensitivity then he or she can realize why relative sensitivity is increasing with wavelength increasing. Because from sensitivity equation, it is seen that sensitivity is inversely related with effective refractive index. As effective refractive index decreases with increasing wavelength, so relative sensitivity increases with increasing wavelength. Again, as the effective refractive index in y polarization direction is higher than x polarization direction, so the relative sensitivity is higher in x polarization direction than y polarization direction. That's why the presented model provides higher sensitivity in x polarization direction than y polarization direction. On account of this, if the proposed sensor is allowed to propagate in x polarization direction, then it will provide better performance to sense sulfuric acid. In this proposed PCF model, the sensitivity increases rapidly from 0.8 to 1.5 μm, and it becomes approximately constant with wavelength change.

The sensor structure provides around 59.5%, 60.2%, 60.8%, 61.5%, 62.2% sensitivity at 1.5 μm wavelength for 0%, 10%, 20%, 30%, 40% H_2SO_4 solution respectively in y polarization direction. Figure 7 also shows same sensitivity characteristic as like Fig. 6. The proposed sensor provides about 60.7%, 61.4%, 62%, 62.7%, 63.4% sensitivity at 1.5 μm wavelength for 0%, 10%, 20%, 30%, 40% H_2SO_4 solution respectively in x polarization direction.

Confinement loss is another important sensing property. The reason is to get better sensing performance; the sensor should have lowest confinement loss. Figure 8 shows confinement loss profile of proposed model.

Figure 8 shows around zero confinement loss from 1 to 1.35 μm and after that confinement loss shows an increasing trend. Again for high concentration of sulfuric acid, confinement loss is seen to be lower. It happens because for increasing sulfuric acid concentration, light confinement becomes higher and confinement loss becomes lower. Confinement loss is found approximately 8.4848×10^{-16}, 3.4858×10^{-16}, 1.9619×10^{-16}, 3.2539×10^{-17}, 1.422×10^{-17} dB/km at wavelength 1.5 μm when 0%, 10%, 20%, 30%, 40% H_2SO_4 solution is placed into the fiber core. For this reason, the proposed PCF model will deliver moderately superior performance for wavelength from 1 to 1.35 μm.

In this work, we also roughly investigated the effective area for the presented sensor and Fig. 9 shows the effective area curve with respect to wavelength variation. Highest effective area is obtained for highest sulfuric acid's concentration and it is logical. Because, when large amount of sulfuric acid is inserted through fiber core, then overall core index increases and on account of this overall sensing area also increases. Around 19 μm^2 effective area is achieved at wavelength 1.5 μm when 40% sulfuric acid concentration is taken as analyte.

In PCF based chemical sensing arena, some researches

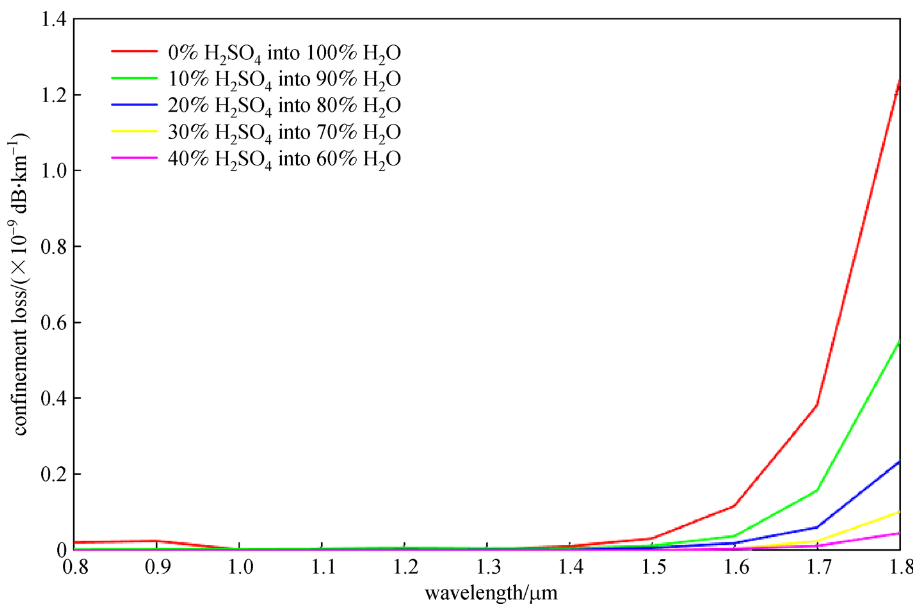

Fig. 8 Confinement loss vs. wavelength for different sulfuric acid concentrations

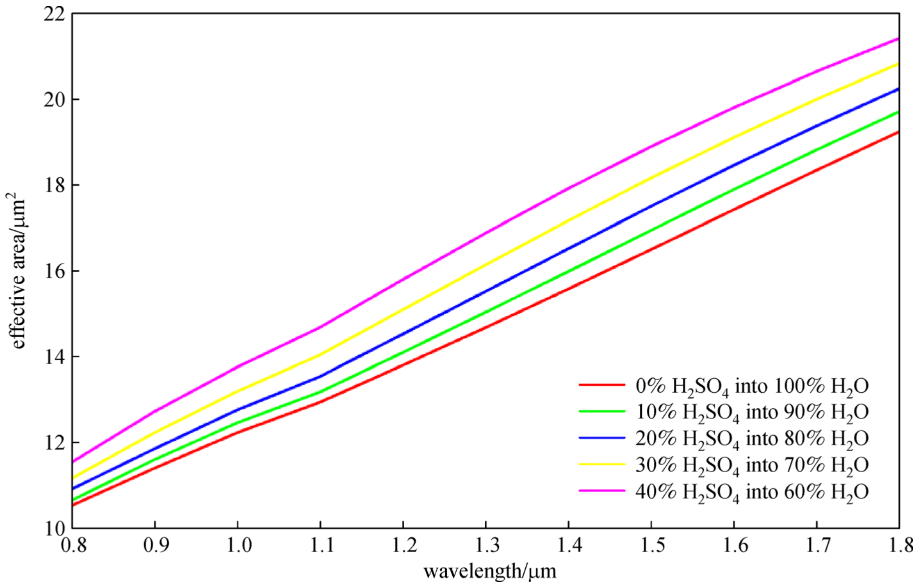

Fig. 9 Effective area vs. wavelength for different sulfuric acid concentrations

Table 4 Comparison of sensitivity, confinement loss and birefringence among the previous research works and the presented work for different liquids at 1.55 μm wavelength

research work	birefringence	confinement loss	relative sensitivity
Ref. [18]	4.90×10^{-4}	0.0001 dB/km	9%
Ref. [19]	2.40×10^{-4}	0.00000025 dB/km	24%
Ref. [21]	1.53×10^{-3}	2.75×10^{-12} dB/km	48%
Ref. [30]	2.16×10^{-4}	0.000000279 dB/km	–
proposed PCF	7.50×10^{-4}	1.422×10^{-17} dB/km	63.5%

also presented almost similar work, though design parameters are different in their model. But some of them are still in proposed level, that's why still we have chance to compete with their results. On account of this, finally, we have shown relative comparison with respect to previous research works on PCFs in Table 4.

5 Conclusion

It is very worthy to sense sulfuric acid concentration precisely while manufacturing different chemicals like hydrochloric acid, nitric acid, sulfate salts as well as drugs. Nowadays, PCF provides outstanding sensing platform for detection of chemical like sulfuric acid. For this reason, a hexagonal PCF sensor model is designed and analyzed for sulfuric acid detection. Relatively high sensitivity, high birefringence with low confinement loss is achieved by this proposed PCF model. The sensor structure provides around 62.2% sensitivity in y polarization direction where approximately 63.4% sensitivity is achieved in x polarization direction for the highest concentration of H_2SO_4 at 1.5 μm wavelength. This PCF model also shows zero confinement loss for wavelength ranging from 1 to 1.35 μm for all solutions of H_2SO_4 and it is found approximately 1.422×10^{-17} dB/km at the wavelength 1.5 μm when 40% H_2SO_4 solution is placed into the fiber core. High birefringence is also achieved and it is observed around 7.5×10^{-4} at the wavelength 1.5 μm for the lowest concentration of H_2SO_4. Also high effective area is obtained for this proposed sensor.

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