Data Article

Dataset of surface plasmon resonance based on photonic crystal fiber for chemical sensing applications

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\textbf{A B S T R A C T}

In this research work a perfectly circular lattice Photonic Crystal Fiber (PCF) based surface Plasmon resonance (SPR) based sensor has been proposed. The investigation process has been successfully carried out using finite element method (FEM) based commercial available software package COMSOL Multiphysics version 4.2. The whole investigation module covers the wider optical spectrum ranging from 0.48\,\mu m to 1.10\,\mu m. Using the wavelength interrogation method the proposed model exposed maximum sensitivity of 9000 nm/RIU (Refractive Index Unit) and using the amplitude interrogation method it obtained maximum sensitivity of 318 RIU\textsuperscript{-1}. Moreover the maximum sensor resolution of 1.11\times10^{-5} in the sensing ranges between 1.34 and 1.37. Based on the suggested sensor model may provide great impact in biological area such as bio-imaging.

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**Specification Table**

| Subject area                          | Sensor                                      |
|---------------------------------------|---------------------------------------------|
| More Specific Subject area            | Surface Plasmon Resonance based biosensor. |
| Types of data                         | Numerical analysis                          |
| How data was acquired                 | Full vectorial finite element method (FV-FEM) based tool COMSOL Multiphysics version 4.2 with circular PML. |
| Data format                           | Raw data, tables, figures.                  |
| Data accessibility                    | Data within the article and GitHub. Link:   |

**Value of the data**

- A PCF based SPR sensors are highly used in clinical diagnosis and the biomedical engineering based devices. The SPR based sensor has been proposed to enhance the performance of the sensor system.
- Derived numerical can assist the engineers, researchers, scientist, those who are especially interested with SPR based chemical.
- The presented simple designs and data analysis can support the researchers to reduce the complexity and implement high robust SPR sensor designs.
- Dataset is highly suitable for the benchmark of different liquid as well as chemical sensing application using PCF based SPR sensor.
- Presented sensor model is experienced with superior performance than the previous existing sensor model.

1. Data

This article demonstrates the implementation of the photonic crystal Fiber (PCF) based sensor with cross sectional view. Table 1 is illustrating the data set for gold thickness of the structure; Table 2 is demonstrating the dataset for PML depth on fiber properties; Table 3 is describing about different chemical area; Table 4 is illustrating the data set for various radius of the center air hole; Table 5 is describing the dataset for different pitch value.

The data which describes above tables are comparable with the articles [1–3].

2. Experimental design, materials and methods

Recently, various kinds of SPR based structures are also proposed [4–6] to obtain the high performance. Fig. 1(a) shows a circular lattice PCF sensor structure of cross sectional view. There have two layers of air holes in this structure where two air holes are missing in each layer. Comparatively two small air holes are placed in the second ring and one air hole is placed in the center. Here in the proposed structure, the distance between center-to-center is defined by the p, the radius of the center air hole is defined by \( r_c \). \( r_c \) is defined as the radius of the small air holes which is equal to \( r_c \). \( r_1 \) is the radius of rest of the air holes and the thickness of the gold layer is defined by \( d_g \). A larger central air-hole \( r_c \) is used to reduce the effective index of the core guided and as a result deteriorate the guidance along the core [7]. The gold film layer is placed at the outside of the fused silica layer where the thickness \( d_g \) of the gold film layer is 35 nm. The analyte layer is placed outside the gold layer which thickness is 0.965 \( \mu \)m. In this raised structure the size of \( r_1 \) is 0.4 \( \mu \)m. Last outer most layers are Perfectly Match Layer (PML) which thickness is 7.2 \( \mu \)m. The back ground layer of the structure is fused silica. Fig. 1(b) and (c) presents the surface mode and at wavelength \( \lambda = 0.70 \mu \)m and \( n_a = 1.37 \) nm.

In this raised structure we used a thin gold layer as an active plasmonic material outside the outermost air holes layer. Since gold is chemically inactive in hydrous atmosphere and represents rich resonance peak shift [8]. An analyte layer is also used outside the gold layer which will help to make a
Table 1
Variations on several Gold thicknesses to observe the modal properties of the proposed PCF the operating wavelength $\lambda = 0.48 \mu m$ to $1.10 \mu m$. The diameter of center air hole at the first layer and other two air hole at the second layer are $r_c = r_2 = 0.2 \mu m$. The rest air holes are denoted by $r_1$ where, $r_1 = 0.4 \mu m$. The air holes inside the ring are organized by maintaining a fixed distance $(p)$ where, $p = 1.8 \mu m$. The thickness $d_g$ of the gold layer, analyte layer and PML layer is $30–40$ nm, $0.965 \mu m$ and $7.2 \mu m$ respectively.

| Gold thickness (nm) | Analyte ($n_a$) | Peak Loss (dB/cm) | Amplitude sensitivity (RIU$^{-1}$) |
|---------------------|-----------------|-------------------|-----------------------------------|
| 30                  | 1.36            | 172.32 (at $\lambda = 0.51 \mu m$) | 240.0451                          |
|                     | 1.37            | 397.06 (at $\lambda = 0.59 \mu m$) |                                    |
| 35                  | 1.36            | 375.49 (at $\lambda = 0.62 \mu m$) | 318.1160                          |
|                     | 1.37            | 700.04 (at $\lambda = 0.71 \mu m$) |                                    |
| 40                  | 1.36            | 424.01 (at $\lambda = 0.72 \mu m$) | 288.9673                          |
|                     | 1.37            | 537.49 (at $\lambda = 0.51 \mu m$) |                                    |

Table 2
Variations of several PML depth to observe the modal properties of the proposed PCF; the operating wavelength $\lambda = 0.48 \mu m$ to $1.10 \mu m$ and gold thickness $35$ nm. The diameter of center air hole at the first layer and other two air hole at the second layer are $r_c = r_2 = 0.2 \mu m$. The rest air holes are denoted by $r_1$ where, $r_1 = 0.4 \mu m$. The air holes inside the ring are organized by maintaining a fixed distance $(p)$ where, $p = 1.8 \mu m$. The thickness $d_g$ of the gold layer, analyte layer and PML layer is $35$ nm, $0.965 \mu m$ and $7.0–7.4 \mu m$ respectively.

| PML depth (µm) | Wavelength (µm) | Analyte ($n_a$) | Peak Loss (dB/cm) |
|----------------|-----------------|-----------------|-------------------|
| 7.0            | 0.56            | 1.35            | 106.17            |
|                | 0.62            | 1.36            | 374.76            |
| 7.2            | 0.56            | 1.35            | 106.34            |
|                | 0.62            | 1.36            | 375.49            |
| 7.4            | 0.72            | 1.35            | 374.81            |
|                | 0.84            | 1.36            | 106.17            |

Table 3
Variations of several chemical area to observe the modal properties of the proposed PCF; the operating wavelength $\lambda = 0.48 \mu m$ to $1.10 \mu m$, gold thickness $35$ nm and PML $7.2 \mu m$.

| Chemical area (µm) | Analyte | Peak Loss (dB/cm) | Amplitude sensitivity (RIU$^{-1}$) |
|--------------------|---------|-------------------|-----------------------------------|
| 0.565              | 1.35    | 106.17 (at $\lambda = 0.56 \mu m$) | 269.8864                          |
|                    | 1.36    | 374.76 (at $\lambda = 0.62 \mu m$) |                                    |
| 0.965              | 1.35    | 106.34 (at $\lambda = 0.56 \mu m$) | 318.1160                          |
|                    | 1.36    | 375.49 (at $\lambda = 0.62 \mu m$) |                                    |
| 1.365              | 1.35    | 106.17 (at $\lambda = 0.56 \mu m$) | 291.3925                          |
|                    | 1.36    | 374.81 (at $\lambda = 0.62 \mu m$) |                                    |

Table 4
Variations of several radius of center air hole to observe the modal properties of the proposed PCF; the operating wavelength $\lambda = 0.48 \mu m$ to $1.10 \mu m$, gold thickness $35$ nm, PML $7.2 \mu m$ and chemical area $0.965 \mu m$.

| Center air hole radius (µm) | Analyte ($n_a$) | Peak Loss (dB/cm) | Amplitude sensitivity (RIU$^{-1}$) |
|-----------------------------|-----------------|-------------------|-----------------------------------|
| 0.1                         | 1.35            | 104.39 (at $\lambda = 0.56 \mu m$) | 290.1938                          |
|                             | 1.36            | 367.89 (at $\lambda = 0.62 \mu m$) |                                    |
| 0.2                         | 1.35            | 106.34 (at $\lambda = 0.56 \mu m$) | 318.1160                          |
|                             | 1.36            | 375.49 (at $\lambda = 0.62 \mu m$) |                                    |
| Without center              | 1.35            | 103.99 (at $\lambda = 0.56 \mu m$) | 289.9285                          |
|                             | 1.36            | 366.34 (at $\lambda = 0.62 \mu m$) |                                    |
fiber structure easier and straightforward for fabrication process. We considered only one fiber core mode in the data set because this core mode is only eligible to provide high performance. On the other side, another mode provides abject performance and is not present for all wavelength $\lambda$ (lambda). That's why we neglect another mode. By following step by step analyzing process the operating selected mode can be achieved.

The following Sellmeier equation \[8\] is used to obtain the refractive index,

$$n^2(\lambda) = 1 + \frac{B_1 \lambda^2}{\lambda^2 - C_1} + \frac{B_2 \lambda^2}{\lambda^2 - C_2} + \frac{B_3 \lambda^2}{\lambda^2 - C_3}$$

where $n$ is denoted refractive index of fused silica that dependent on wavelength ($\lambda$), $\lambda$ is the wavelength in $\mu$m. $B_1$, $B_2$, $B_3$, $C_1$, $C_2$ and $C_3$ are denoted the Sellmeier constants. The values of corresponding constants are respectively 0.69616300, 0.407942600, 0.897479400, 0.00467914826, 0.0135120631, and 97.9340025 for fused silica.

The following Drude–Lorenz model \[9\] is used to obtain the dielectric constant of the gold,

$$\epsilon_{Au} = \epsilon_\infty - \frac{\omega_p^2}{\omega(\omega + j\gamma D)} - \frac{\Delta \epsilon \cdot \Omega_L^2}{\omega^2 - \Omega_L^2 + j\pi \Gamma \omega}$$

where the permittivity of gold is denoted by $\epsilon_{Au}$, $\epsilon_\infty$ is the permittivity at high frequency that has a value of 5.9673, $\omega$ is the angular frequency that is defined as $\omega = 2\pi c / \lambda$, $c$ is the velocity of light in vacuum, $\omega_D$ is denoted the plasma frequency, the damping frequency is denoted by $\gamma D$, where $\omega_D = 4227.2\pi$ THz, $\gamma D = 31.84\pi$ THz and weighting factor $\Delta \epsilon = 1.09$. The spectral width $\Gamma L = 209.72\pi$ THz and oscillator strength $\Omega_L = 1300.14\pi$ THz respectively.

The following equation \[10\] is used to obtain the sensor’s performance,

$$\alpha \left[ \frac{dB}{m} \right] = 8.686 \times k_0 \cdot Im[n_{eff}] \times 10^4$$

Table 5

Variations of several pitch value to observe the modal properties of the proposed PCF; the operating wavelength lambda ($\lambda$)=0.48 $\mu$m to 1.10 $\mu$m, gold thickness 35 nm, PML 7.2 $\mu$m, chemical area 0.965 $\mu$m and radius of center air hole 0.2 $\mu$m.

| Pitch ($\mu$m) | Analyte ($n_a$) | Peak Loss (dB/cm) | Amplitude sensitivity (RIU$^{-1}$) |
|---------------|----------------|-------------------|-----------------------------------|
| 1.50          | 1.35           | 276.85 (at $\lambda = 0.55 \mu$m) | 231.6415 |
| 1.36           |                | 807.90 (at $\lambda = 0.61 \mu$m) |                |
| 2.00          | 1.35           | 106.34 (at $\lambda = 0.56 \mu$m) | 318.1160 |
| 1.36           |                | 375.49 (at $\lambda = 0.62 \mu$m) |                |
| 2.50          | 1.35           | 52.61 (at $\lambda = 0.57 \mu$m) | 261.3937 |
| 1.36           |                | 175.49 (at $\lambda = 0.62 \mu$m) |                |

Fig. 1. The cross sectional end faced view of the proposed PCF based SPR sensor.
where \( k_0 = \frac{2\pi}{\lambda} \) is denoted the number of free space, operating wavelength is denoted by \( \lambda \) and the imaginary part of the effective refractive index denoted by \( \text{Im}(n_{\text{eff}}) \).

To obtain the sensitivity of the PCF-based SPR sensor the following formula [11] is used,

\[
S = \frac{\Delta \lambda_{\text{peak}}}{\Delta n_a} = \frac{\Delta n_a}{C_0/C_1} \quad \text{RIU}
\]

\(
\Delta \lambda_{\text{peak}}
\)

is used to indicate the distinction of wavelength peak shifts and \( \Delta n_a \) is used to indicate the difference of analyte refractive index RI.

To obtain the resolution of the raised structure the following formula [12] is used,

\[
R(\text{RIU}) = \frac{\Delta n_a}{\Delta \lambda_{\text{min}}/\Delta \lambda_{\text{peak}}}
\]

\(\Delta n_a = 0.01, \Delta \lambda_{\text{min}} = 0.1 \text{ nm}, \text{ and } \Delta \lambda_{\text{peak}} = 90 \text{ nm}; \text{ as a result a high value of sensor resolution is obtained as high as } 1.11 \times 10^{-5}.\)

The following formula [13] is used to obtain the amplitude sensitivity,

\[
S_A(\lambda) \left[ \text{RIU}^{-1} \right] = -\frac{1}{\alpha(\lambda, n_a)} \frac{\partial \alpha(\lambda, n_a)}{\partial n_a}
\]

where \( \alpha(\lambda, n_a) \) is denoted the overall propagation loss at a specific refractive index (RI) of analyte and \( \partial \alpha(\lambda, n_a) \) is indicated the difference between the two loss spectra.

Fig. 3(a) shows the consequent loss spectra for different gold layer thickness at analyte RI of 1.36 and 1.37 as described in Table 1. From this analysis we can see that the proposed structure provide highest...
loss for gold thickness 35 nm. On the other hand, Fig. 2(b) presents the corresponding amplitude sensitivity with the variation of gold thickness. It easily clarify that the proposed structure is also provides highest amplitude sensitivity for gold layer thickness 35 nm.

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Transparency document. Supporting information

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Appendix A. Supporting information

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