Plasmonic sensor based on microstructure PCF: performance analysis with outside detecting approach

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Abstract
In this paper, a novel microstructure photonic crystal fiber (MC-PCF)-surface plasmon resonance sensor is presented and developed using the finite element method with perfectly matched layer boundary condition. The sensor performance in terms of wavelength sensitivity (WS), amplitude sensitivity (AS), and figure of merit (FoM) is quantitatively examined using an external sensing technique with an optimal thickness of 40 nm of chemically stable gold. Finer mesh analysis is also used for modal analysis. At this optimized gold thickness, the highest recorded WS of 92,000 nm per RIU and AS of 1080 per RIU at a detecting range of 1.33–1.38 RIU are obtained. Within this detecting range, the sensor also has a strong linear fit and a FoM of 348.15 per RIU, respectively. Because of its high sensitivity and FoM, the suggested sensor might be a viable competitor in detecting the analyte refractive index. Finally, to demonstrate the performance capability of our proposed sensor, all performance parameters were compared to previously published studies.

Keywords FOM · Sensitivity · SPR · PCF · Microstructure · PML

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1 Introduction

The surface plasmon resonance (SPR) based microstructure photonic crystal fiber (MC-PCF) sensors have become intensively research topic now a days because of its simplicity, cost effective operation, high sensing ability, compactness, remote sensing capability, less fabrication complexity, high detecting range and high sensing accuracy (Rifat et al. 2017). The working methodology of the SPR-MC-PCF sensor is based on the interaction between the incident light which is applied to the analyte/gold layer interface and metal thin film surface (Rifat et al. 2017; Haque et al. 2018). As per literatures, the analytical ideology of SPR sensing approach was firstly come to the light by Rithie et al., in the 1950s (Hossain et al. 2020b). After then, the application based real 3D design based on prism comprised model was first developed and applied in real life sensing application by Kretschmann and Otto in 1968 (Hossain et al. 2020c). In Kretschmann and Otto introduced configuration, the two major excitation processes of surface plasmon waves (SPW) were discussed that were the attenuated total reflection (ATR) in prism coupler based and the diffraction grating based (Hossain et al. 2020c; Rifat et al. 2017a). Since, the prism coupler-based method not only needs larger structure size but also has less sensitivity (Sakib et al. 2020), the PCF fiber based method is widely utilized. The PCF-SPR configuration is consisted a circular glass fiber with distributed air hole inside the fiber (Hossain et al. 2020b). The functionality of the air hole is to behave as low-density medium for light energy. When light is incident at the analyte/gold interface, the total internal reflectance has been occurred and generated a surface plasmon wave (SPW) which propagates along the gold layer surface (Hossain et al. 2020c). At the moment of incident of polarized light energy into the metal film, it releases free electron which is actually resulted for this SPW (Hossain et al. 2020c). When the propagation constant of SPW and incident light is identical, then a significant amount of energy is transferred from incident light energy to the free electrons of metal. At this point surface plasmon resonance event (SPRE) has been occurred and at this point a sharp peak of confinement loss is noticeable (Rifat et al. 2017a). The wavelength at which SPRE occurs, is called SPR wavelength (Rifat et al. 2017a). The unknown analyte can be detected and sensed observing this loss peak. In most of the fabrication designs, the background of PCF core is filled by fused silica because of its high sensitivity capability at low operating temperature (Sakib et al. 2020). The noble plasmonic material selection is a crucial object for improving sensing performance (Sakib et al. 2020), therefore, the researchers have used several materials such as gold, silver, titanium di-oxide (TiO2), aluminum etc. (Hossain et al. 2020b) for their modeling. Though silver (Ag) has very high resonance peak, it is not suitable in outside detecting approach because of exhibiting chemical instability and rapid oxidation (Szunerits et al. 2013). On the other hand, gold is utilized typically due to its highly chemically stable in nature and good adhesive property (Hossain et al. 2020b). Beside the advantages of external coating film, the addition of such film causes extra fabrication cost. So, for the chemical stability and low fabrication cost, gold is mostly preferred plasmonic material (Hossain et al. 2020b, c; Sakib et al. 2020). There are several sensing approaches, among them the outside sensing approach with incorporating gold optimized thickness is advancing more in biomolecular science and technological applications, for example, biomolecular sensing and detecting (Mollah et al. 2020; Lu et al. 2015; Hossain et al. 2021, 2020a, b, c), temperature sensing (Mollah et al. 2020), pollution sensing (Lu et al. 2015), environmental sensing and detecting (Lu et al. 2015), water testing (Lu et al. 2015), antigen–antibody interaction (Hossain et al. 2021), medical diagnosis (Hossain et al. 2020a) etc.
Owing to its numerous advantages, several structures of the PCF based SPR sensors have been introduced till date. In literature (Hossain et al. 2020b), M. B. Hossain, et. al. proposed a numerical analysis of gold coating based quasi D-shape dual core PCF SPR sensor which shows WS of 15,000 nm/RIU and AS of 230/RIU. This paper has good WS but suffers from low AS. M. N. Sakib et.al. in literature (Nazmus et al. 2019), proposed a high-performance dual core D-shape PCF-SPR sensor modeling employing gold coat. The proposed sensor shows a highest WS of 8000 nm/RIU, wavelength resolution of 1.25 × 10⁻⁵ RIU, a highest AS of 700 per RIU, amplitude resolution 1.7857 × 10⁻⁵ RIU and a figure of merit (FoM) of 138 per RIU owing to ARI altering from 1.47 to 1.48 RIU. M. B. Hossain, et al. in literature (Biplob et al. 2020) proposed a silver coated hollow-core PCF sensor was reported. This sensor reduced fabrication difficulties but shows less WS of 21,000 nm per RIU. Very recently, M. N. Sakib et al. in Nazmus et al. (2021) proposed a microstructure PCF based SPR sensor with having WS of 75,000 nm/RIU and AS 480/RIU. Though this paper has significantly high WS, it suffers significantly low AS.

In this article, a novel very high sensitivity-based microstructure-based PCF-SPR sensor is proposed where optimized gold thickness as external sensing approach is utilized to improve sensor performance. The proposed sensor shows a very high WS of 92,000 nm/RIU, and AS of 1080 per RIU for a wide sensing range of 1.33 RIU to 1.38 RIU. The performance is evaluated numerically by combing the finite element method/FEM with Perfectly Matched Layer (PML) following the boundary condition of scattering case. The main property of a PML is that incident waves upon the PML from another medium do not reflect at the interface. This property allows the PML to strongly absorb outgoing waves from the inward of a computational region without reflecting them back into the inside. Modal analysis is performed using finer mesh analysis. The superior sensor performance has been ensured by utilizing the newly proposed model along with optimized gold thickness of 40 nm.

2 Proposed sensor configuration

The schematic 3d cross-sectional presentation of the proposed microstructure PCF-SPR sensor is shown Fig. 1. In the proposed configuration, there are two semicircular lattice, the outer ring is composed with four missing air holes. These air holes are combinedly used to behave as low-density medium for light energy and generate very high evanescent electromagnetic field in order to perform fast SPRE.

Figure 1 describes the core mode of x-polarization and SPP mode of y-polarization in where the SPW is propagated along x-indices (Nazmus et al. 2021). At SPRE point, as aforementioned, the energy is transferred from fundamental x-polarized core mode to fundamental x-polarized SPP mode. From Fig. 1, it is clear that the proposed architecture shows a symmetric configuration. There are many advantages of such symmetric configuration such as sharp resonance peak, minimum reflection, etc. at SRRE (Nazmus et al. 2021). The length between two adjacent air holes is known as pitch (Λ). In this paper, a standard pitch of 2 um which is reported in Nazmus et al. (2021), is utilized. The diameter of the outer ring air hole is kept as large as 0.78 Λ and on the other hand, the diameter of the inner ring air hole is kept 0.57 Λ (Nazmus et al. 2021). Since the main background is fused silica, therefore, it is needed to know the RI of the silica material which can be calculated by well-known Sellmier equation as given below (Biplob et al. 2020; Nazmus et al. 2021):
where \( n(\lambda) \) is the wavelength dependent analyte refractive index measured in \( \mu m \), \( B_1, B_2, B_3, C_1, C_2, \) and \( C_3 \) are the Sellmier equation constant utilized from Nazmus et al. (2021). Since a very thin film of gold about 40 nm is needed for external coating, chemical vapour deposition (CVD) method is usually used to produce this coat. The dielectric function of Au is received from Drude-Lorentz model (Akter et al. 2019; Rifat et al. 2017b). The dielectric constant of the gold is also a frequency dependant parameter which can be expressed by Drude-Lorentz model as follows (Akter et al. 2019; Rifat et al. 2017b):

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

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\[
 \varepsilon_{Au} = \varepsilon_{\infty} - \frac{\omega_D^2}{\omega(\omega + j\gamma_D)} - \frac{\Delta \varepsilon}{\omega^2 - \Omega_L^2} + j\Gamma_L \omega
\]

where, the permeability and permittivity of Au are denoted by \( \varepsilon_{Au} \) and \( \varepsilon_{\infty} \), respectively. At very high frequency the \( \varepsilon_{\infty} \) can be chosen to 5.9673. The other parameters for the designing purpose are taken for (Rifat et al. 2017b). The thickness of unknown analyte is chosen to 1.5 \( \mu m \) and 1.5 \( \mu m \) of PML layer with sensing scattering boundary condition (SBC) is used as boundary condition which is 10% of total PCF diameter. The FEM based mode solver COMSOL Multiphysics platform is used to model and investigate the proposed sensor performance and the associated computation is performed by MATLAB platform.

### 3 Simulation results and discussions

The performance of the proposed sensor is studied by taking into account the total number of horizontal elements 20,256, the number of vertex elements 128, the number of boundary elements 1628 and each element step size of 0.7988 nm. To investigate a sensor’s sensitivity, we must first collect the confinement loss curves with respect to different incident wavelengths. The confinement loss is achieved by utilizing the well-known formula given
In Nazmus et al. (2021; Akter et al. 2019; Rifat et al. 2017b; Mahfuz et al. 2020; Anik et al. 2021):

\[ \alpha(\text{dB/cm}) = 8.68 \times k_0 \text{Im}(n_{\text{eff}}) \times 10^4 \]  

(3)

In Eq. (3), \( \text{Im}(n_{\text{eff}}) \) is the imaginary part of the analyte RI for core mode propagation, \( k_0 \) is the number of waves, and \( \lambda \) is the operating wavelength of incident light (Islam et al. 2018). Figure 2a depicts the confinement loss curve, whereas Fig. 2b, c, and d depict the x polarized core mode, y polarized core mode, and SPP mode, respectively. From Fig. 2a, it is shown that the curve of confinement loss is almost symmetrical with respect to the SPR wavelength, because, before reaching SPR wavelength, more energy is transferred from fundamental incident light to SPW and it is maximum at SPR wavelength, after crossing SPRE point, if the wavelength of incident light is further increased then also the amount of transferring energy reduces. It is clearer that the peak point of confinement loss is more sharp which indicates the proposed sensor advantages, for example, more accurate sensing applications has been obtained. From Fig. 2a, it has been shown that at \( n_a = 1.354 \) RIU with \( t_g = 40 \) nm, the SPP core mode real and x-polarized core real intersect to each other, and this is the SPRE point. By observing this point shift, the unknown ARI can be sensed.

As stated above, the wavelength at SPRE point is called SPR wavelength. The wavelength at which the modes of two cases are intersected is also called phase matching wavelength and a sharp resonance peak is happened at that corresponding wavelength. In case of the resonance wavelength, the maximum energy is transferred to the plasmonic mode from the from the core mode.

**Fig. 2**  
(a) Matching relation of dispersion phase between the mode of the fundamental core and SPP, (b) x-polarized core mode, (c) y-polarized core mode, (d) SPP mode at \( n_a = 1.445 \) and \( t_g = 40 \) nm.
To investigate sensor performance, one of the key parameters is confinement loss curve which is used to improve sensor performance. The confinement loss curve is also used to compute wavelength sensitivity as well. The calculation of confinement loss curve is done by using the well-known as given in Eq. (3). As shown in Fig. 3a, the resonance peak is shifted to rightward with respect to increase analyte to different wavelength due to different analyte profile. So, it can be concluded that if ARI increases, the SPRE point also increase. After computing confinement loss curve, the calculation of sensor WS has been taken place. Therefore,

Fig. 3  a Confinement loss profile, and b corresponding AS with respect to incident wavelength for a detecting range of 1.33RIU to 1.38 RIU, with $\Lambda = 2 \mu m$, $d_s = 0.57\Lambda$, $d_l = 0.78\Lambda$, and $t_g = 40$ nm
it can be made a conclusion that the deviation of the analyte to rightwards. profile of RI is one of the significant ways in analyzing the output of the offered design which is measured by:

\[ S_{\lambda}(nm/RIU) = \frac{\Delta \lambda_{\text{peak}}}{\Delta n} \]  

(4)

In Eq. (4), \( \Delta \lambda_{\text{peak}} \) is the variation of peak wavelength with respect to ARI, \( \Delta n \) is the change of ARI. The one of the simplest ways to compute wavelength sensitivity is to observe the shift of peak wavelength with respect to the change of ARI. For the proposed sensor, the confinement loss profile with respect to different wavelength is shown in Fig. 3a. By applying wavelength interrogation method described in Eq. (4), the proposed sensor offers maximum WS of 92,000 nm per RIU. This is the highest value of WS in the literature, as far the knowledge gathered from literatures survey.

Another important performance indicator parameter is amplitude sensitivity which can be obtained by adopting amplitude interrogation procedure. In this approach, the AS of the proposed sensor can be calculated by the following expression (Nazmus et al. 2021):

\[ S_A(\text{RIU}^{-1}) = \frac{1}{\alpha(\lambda, \eta)} \times \frac{\partial(\lambda, \eta)}{\partial \eta} \]  

(5)

The loss of propagation and loss of gap can be denoted by \( \alpha(\lambda, n) \), and \( \delta(\lambda, n) \), respectively. The loss of propagation and loss of gap both are the wavelength and ARI dependent parameters. The AS for a detecting range of 1.33 RIU to 1.38 RIU are in Fig. 3b with respect to different wavelength. It is clearly shown from Fig. 3b that the maximum AS is found 1080 per RIU at 0.75 um.

The figure of merit (FoM) or the signal to noise ratio (SNR) is another performance parameter of SPR sensor. A good sensor should have high FoM. If a sensor has high FoM, it means this sensor has high capability of detecting unknown analyte. The FoM is inversely proportional to the full width half maxima (FWHM) and directly proportional to the WS. Since the proposed sensor shows very high WS, therefore, it has significantly high FoM. The FoM can be calculated as (Nazmus et al. 2021):

\[ \text{FOM} = \frac{\text{Sensitivity (nm/RIU)}}{\text{FWHM}} \]  

(6)

The FoM spectra with respect to ARI is shown in Fig. 4, where it is found that if wavelength increases, the FoM also increases because at higher wavelength the WS is higher which is clearly shown from confinement loss curve. Equation (6) reveals that, higher FoM is achievable by keeping FWHM as small as possible. In Fig. 4, the FoM profile is calculated for a detecting range of 1.33 RIU to 1.38 RIU. It is visible that with increasing analyte refractive index (na), the sensitivity is increasing but the and the FWHM reduce as the narrow resonance peak is observed. Therefore, the maximum FoM is found 348.15 RIU\(^{-1}\) at ARI of 1.38 RIU.

A good sensor should have high linearity property. The fitting property of the proposed sensor is demonstrated in Fig. 5, with analyte RI variation ranging 1.33 to 1.38 RIU. First at all, we imposed the following fitting equation to describe sensor fitting characteristics:

\[
\begin{align*}
\text{PolynomialFit : } y &= 125x^2 - 334.89x + 224.97; \text{ where, } R^2 = 0.998 \\
\text{LinearFit : } y &= 6.3571x - 7.87; \text{ where, } R^2 = 0.8196
\end{align*}
\]  

(7)
From Fig. 5, it is shown that the proposed sensor shows high linear property both for linear and polynomial fitting. The R square ($R^2$) value is used to present a sensor how much it has linearity. The $R^2$ value for linearity fitting is found 0.8196, whereas, for polynomial fitting is 0.998. In Eq. (7), $y$ indicates the resonance wavelength and $x$ denotes the analyte’s RI.

Lastly, in this paper, the performance of the proposed sensor is compared with the reported works. The performance comparison study is tabulated in Table 1. Table 1 shows that the proposed sensor has better performance in terms of AS, WS, linearity and FoM.

### 4 Conclusions

In this paper, a high-performance microstructure PCF-SPR sensor is proposed, and numerically developed, in where gold is used as plasmonic material. Sensor performance parameters such as amplitude sensitivity, wavelength sensitivity and figure of merit are investigated by adopting finite element method based solver platform COMSOL Multiphysics software. Numerical results show that the proposed sensor exhibits maximum wavelength
sensitivity of 92,000 nm/RIU which is ever best reported numerical result. The proposed sensor also shows high amplitude sensitivity of 1080 per RIU and high figure of merit of 348.15 per RIU, respectively.

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