Design and Simulation of Surface Plasmon Resonance Sensors for Environmental Monitoring

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Abstract. In this work a Surface Plasmon Resonance (SPR) sensor based on Photonic Crystal Fiber (PCF) infiltrated with water samples has been proposed. To accurate detection of the sample properties, gold is used as plasmonic material. The air holes of PCF has been infiltrated with water samples, the optical properties of these samples has been taken from samples collected from Al-Qadisiya and Wathba lab. (east Tigris, Wathba, and Al-Rasheed) water projects at Baghdad- Iraq. Finite Element Method (FEM) has been used to study the sensor performance and fiber properties. From the numerical investigation we get maximum sensitivity circa 164.3 nm/RIU in the sensing range of 1.33 (of STD water) to 1.3431 (of river sample). The proposed sensor could be developed to detect various high refractive index (RI) chemicals like the heavy metals in water.

Keyword. SPR; FEM; PCF; Optical sensing and sensors; environment monitoring

1. Introduction
Surface plasmon could be define as plasma oscillations supported by metal dielectric interface. The oscillations of charge density along this interface are define as surface plasma oscillations mode for the quantized oscillation of these modes; the quantized oscillations of the oscillated modes called surface plasmon mode. Theses modes are joined to longitudinal electric field; the field intensity suffering exponential decay in metal and dielectric materials. Due to this decay, the field intensity has maximum value at the metal- dielectric interface. Maxwell’s equations for metal dielectric Refractive Index (RI) distribution are used to study the properties of the surface plasmon and decay of this decay, the origin of the phenomenon of Surface Plasmon Resonance (SPR) began theoretically studied in 1907 by Zenneck [1, 2].
Surface Plasmon Resonance sensors widely used in field of detection chemical and biological components which is very helpful in fields like environmental monitoring, food safety and medical diagnostics, with high sensitivity also no molecular labels are used [3]. Although, these sensors commercially available but they used only in laboratory due to their high cost and large size. So, to solve this problem a need for smaller and cheaper SPR sensor become a very important point, this is achieved by using optical fiber-based SPR sensors [4]. These sensors are based on different types of fibers, such as Single Mode Fiber (SMF), Multimode Fiber (MMF) and Photonic Crystal Fiber (PCF) [5].

In this work SPR-sensor based on PCF has been submitted, PCF’s are special type of fibers, which have a periodic array of air holes with different shape, size, and distribution running along the entire length of the fiber. The existence of these holes allow controlling fiber properties like chromatic dispersion, high birefringence and non-linearity, which is not suitable in ordinary fibers [6, 7]. In addition, these holes could be infiltrated with different liquids and gases, which give them very good advantages in sensing applications [8], ‘figure 1’ shows different types of PCFs.

The SPR-PCF sensors working principle is based on the evanescent field that is generated due to the propagation of light through the region of core-cladding interface getting interaction between light and plasmonic surface. This lead to changing the RI of the infiltrated analyte and thus changing the RI of the guided light mode, so the resonant wavelength change and lead to detect the particles or molecules by measuring the shifting in resonant wavelength [9]. Gold and Silver are widely used as an active plasmonic materials, although Silver is easily oxidize but it commonly used than Gold due to its high conductivity and sharp resonant peak [10]. In this work Gold has been chosen as a plasmonic material to prevent the oxidation of Silver due to the infiltration of air holes with water samples.

![Figure 1. Some typical structures of MOFs (A) Solid Core-PCF, (B) Suspended core PCF; (C) Hollow Core-PCF, and (D) Kagomé HC-PCF [7].](image)

2. Simulation treatment
The submitted simulation has two air holes rings arranged in hexagonal shape as it shown in ‘figure 2’. Light will be propagate in the air holes area, the SPR-PCF has hole to hole spacing (\(\Lambda\)) circa 1.2 \(\mu\)m, air hole diameter (\(d\)) 4 \(\mu\)m, normalized air hole size (\(d/\Lambda\)) is 3.3, and core diameter (\(r\)) 8 \(\mu\)m, the thickness of the gold layer (\(t\)) is about 2 \(\mu\)m. The refractive index of the fiber material is assumed 1.45.
The analysis of this model has been done by Finite Element Method (FEM) with Perfectly Matched Layer (PML) boundary condition. The FEM has allowed the successful investigation of experiment the characters of mode and calculating the plasmonic mode complex propagation constant.

The complex formula of FEM is very helpful, to evaluate the fiber leakage or confinement losses, because of the holey region of fiber which is consists of finite number of air holes, the eigen value equation can be derived from the Maxwell equations as in equation (1) [11]:

\[ \nabla \times (\mu_r^{-1} \nabla \times \vec{E}) - k_0^2 \varepsilon_r \vec{E} = 0 \]  

(1)

Where \( \vec{E} \) is the electric field, \( k_0 \) is the wave number in vacuum, and \( \varepsilon_r \) and \( \mu_r \) are the dielectric permittivity and magnetic permeability tensors, respectively. The eigen values are \( \beta/k_0 \) the effective indices \( n_{eff} \), and the eigen vectors are the electric field components \( (E_x, E_y, E_z) \) [11].

The modal analyses have been applied on the cross section in the x-y plane of the SPR sensor when the wave is propagating in the z direction. The SPR-PCF cross-section in the transverse X – Y plane is divided into triangular elements with different shapes, sizes, and refractive indices by selecting suitable mesh.

PCF’s considers as a single material fiber, they usually made of pure silica and they has the finite width of the cladding structures so they suffering from type of losses called the confinement losses or leakage losses \( L_c \); \( L_c \) in dB/m is given by [12]:

\[ L_c = -20 \log_{10} e^{-k_0 \mu \rho [n_{eff}]} = 8.686 \mu \rho \mu [n_{eff}] \]  

(2)

Where, \( k_0 \) free space propagation constant, and \( \mu \rho \) is the imaginary part of the complex effective refractive index \( n_{eff} \).

In this simulation, the Drude-Lorentz model will be used to study the dielectric constant of gold as it clear as in equation (3) [13]:

\[ \varepsilon_m = \varepsilon_\infty - \frac{\omega_0^2}{\omega (\omega + j \Gamma_D)} - \frac{\Delta \varepsilon \Omega_L^2}{(\omega^2 - \Omega_L^2) + j \Gamma_L \omega} \]  

(3)

Where \( \varepsilon_m \) gold permittivity, \( \varepsilon_\infty \) gold permittivity in the high frequency, \( \Delta \varepsilon \) is the weighting and equal to 1.09, \( \omega \) is the guided light angular frequency, \( \omega_D/2\pi = 2113.6 \) THz is the plasma frequency, \( \Gamma_D/2\pi = 15.92 \) THz is the damping frequency, \( \Omega_L/2\pi = 650.07 \) THz and \( \Gamma_L/2\pi = 104.86 \) THz are the frequency and spectral width of the Lorentz oscillator.

3. Simulation results
To analyze the sensor characteristics, the air holes of the PCF is infiltrated with different samples of water, the optical characteristics of these samples are measured from real water samples collected from Al-Qadisiya and Wathba lab’s water projects with wavelength range (0.6-1.6) μm.
FEM solver has been used to numerically simulate and investigate the designed model, the core-guided modes and plasmonic mode SPR-PCF. The single mode Gaussian distribution output of selected wavelength are illustrated in ‘figure 3’.

The resonant curves for different water samples refractive indices (na1 = 1.33, na2 =1.3433, and na3 =1.3431) has been studied through investigate coupling properties of the sensor as it illustrated in ‘figure 4’. The phase-matching wavelength condition occur when the real part of effective refractive index of the core-guided mode and that of the plasmonic mode intersect. From figure 4 the loss spectra of the core guided mode could be noticed which is mean that the largest energy transmission from the core guided mode to the plasmonic mode. Therefore, the intersections of the line of core mode and SPR mode represent the resonant wavelength. The resonant wavelengths for samples 1, 2, and 3 is 1.238, 1.399, and 1.41 μm respectively as it is shown in ‘figure 5’.

| λ=0.6μm |      |      |
|---------|------|------|
| STD- Water | Sample 1 | Sample 2 |

Core mode

| λ=1.6 μm |      |      |
|---------|------|------|
| STD- Water | Sample 1 | Sample 2 |

Core mode
SPP mode

**Figure 3.** Single mode Gaussian distribution output of fundamental core and SPP mode for selective wavelength (0.6 and 1.6) µm.

The submitted sensor has resonant features through the depending of the resonant wavelength on the RI of the infiltrated liquid; the sensitivity is defined in the following equation [14]

\[
S_{\omega} = \frac{d\omega_{\text{peak}}(n_{\omega})}{dn_{\omega}}
\]

The maximum sensitivity is 164.3 nm/RIU in range of RI 1.33 (STD water), 1.3431 (river sample) had been achieved.

**Figure 4.** Calculated loss spectrum (blue line) core and SPP mode dispersion relation for water with RI’s (a) (1.33), b (1.3433), and c (1.3431).

**Figure 5.** Resonant Wavelength for all samples.
4. Conclusion
Surface Plasmon Resonance sensor based on Photonic Crystal Fiber (SPR-PCF) coated with Gold layer and air holes filled with water samples has been submitted in this work. By finding the resonant wavelength or the peak of the transmission loss spectrum corresponding to the resonant wavelength of the SPR sensor we can detect identified the filled analyte. The sensor parameters of the fundamental mode had been studied by employing the FEM, The maximum sensitivity is 164.3 nm/RIU in the sensing range of 1.33 (STD water) –1.3431 (river sample) is obtained. Also it is possible to introduce the analytes refractive index range from 1.33 to 1.3431, which is infiltrated into the hole of the proposed sensor. Because of this high sensitivity this technique very recommended to be used for sensing applications in chemical and biological fields like detect the heavy metals in water in the field of environment monitoring.

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