Design and simulation of localized surface plasmon resonance-based fiber optic chemical sensor

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Abstract. In this work, localized surface plasmon resonance based fiber optic (LSPR-FO) sensor utilizing gold nanoparticles (Au NPs) with different sizes is theoretically constructed and analyzed. Three layers (fiber core, Au NPs, and the Analyte) configuration designed by using the matrix method. Performance parameters such as sensitivity, signal to noise ratio, the figure of merit, and resolution of the sensor are evaluated for each size of Au NPs. As a result, sensitivity and resolution exhibit no change with Au NPs size change while the signal to noise ratio and figure of merit decrease as Au NPs size increase. This work shows that the optimized LSPR-FO sensor may have highly promising applications in chemical sensing.

Keywords: Chemical sensor. Localized surface plasmon resonance, Optical fiber.

1. Introduction

The present paper deals with the study of a (LSPR-FO) sensor. LSPR generated from the coupling of surface plasmons with evanescent light, can be used as a sensing technique, with a view to optimize LSPR-FO sensor sensitivity, a lot of researchers have studied coating substances on the surface of the core LSPR-FO sensor such as; Indiums tin oxide (ITO), silver (Ag) and gold (Au) that considered individually[1, 2]. The wavelength interrogation technique utilizes to evaluate LSPR sensor. Generally, an evanescent field is essential for LSPR-FO sensors to produce surface plasmon waves (SPW) at the metal nanoparticles interface as well as the surrounding area [3]. The intensities of LSPR and the noble metal nanoparticles (NPs) wavelengths are mostly considered for their size, shape, NP substance and the refractive index of the surrounding area [4-7]. The higher intensity of LSPR-FO sensor related to the bigger sizes of the NPs [8], and increases particles coverage of the surface [9]. The significance of NPs density on the surface of optical fiber related to the effect of NPs instability that may change the shape of resonance spectra and minimize the measurements accuracy of LSPR-FO sensor [10]. Many studies have been tried to improve the performance of the LSPR-FO sensors. Jiang et al [11], presented a new LSPR sensor based on the U-bent plastic optical fiber (U-POF). The graphene and Ag NPs were forming the film. The graphene improves the sensitivity of the LSPR-FO sensor and prevent the oxidation of the metallic thin. Bae et al [12], suggest a new techniques to enhance the signal to noise ratio (SNR), that consider as important characteristic of the LSPR-FO sensor. First technique increases sensor intensity through increasing the Au NPs size by means of Au capping. Second try, it minimizes the refection by means of increasing surface roughness to minimize the background signal of the sensor. In this paper, a proposed LSPR-FO chemical sensor has been simulated and theoretically studied to obtain optimized sensor with a high sensitivity and resolution.
2. Methodology

According to the principle of total internal reflection (TIR) in an optical fiber and Kretschmann’s configuration [13] a chemical sensor based LSPR is designed. The proposed design consisting of a fiber core, NPs layer (Au NPs) with different sizes, sensing medium (chemical samples) is considered as shown in Fig. 1.

Figure 1: Au NPs deposited on the unclad portion of the Optical Fiber.

Moreover, the plastic cladding that surrounding the core of a step index multimode core fiber (Numerical aperture = 0.24 and core diameter = 600μm) is eliminated after that coated by thin layer of Au NPs. Lastly covered via sensing area. To analyze the (LSPR-FO) sensor a spectral interrogation technique is used. The light launched from a source into the terminals of the optical fiber while, the transmitted light detected at the end of the fiber by using optical spectrum analyzer (OSA). Finally, a sharp dip is appeared in the power of the transmitted signal at the resonance wavelength. The resonance wavelength is based on the refractive index of the sensing area.

2.1. LSPR-FO fundamental media

The LSPR-FO system consists of three fundamental media:

1st Medium: the silica core of optical fiber: The refractive of this medium indicated by \( n_c \). The calculation of \( n_c \) obtained from the dispersion relation of fused silica given by the equation (1) [14]:

\[
n_c(\lambda) = C_0 + C_1 \lambda^2 + C_2 \lambda^4 + \frac{C_3}{(\lambda^2 - a)^2} + \frac{C_4}{(\lambda^2 - a)^3} + \frac{C_5}{(\lambda^2 - a)^5}
\]

(1)

Where the coefficients \( C_0, C_1, C_2, C_3, C_4, C_5 \) and \( a \) are numerical values given as [14]:

\[
\begin{align*}
C_0 &= 1.4508554 \\
C_1 &= -0.0031268 \\
C_2 &= -38.1 \times 10^{-6} \\
C_3 &= 0.0030270 \\
C_4 &= -77.9 \times 10^{-6} \\
C_5 &= 1.8 \times 10^{-6} \\
a &= 0.035.
\end{align*}
\]

2nd Medium: The metallic layer: This layer is of thickness \( d \) from Drude model, the dielectric function of the metallic media given by [15]:

...
Where $\lambda_c$ and $\lambda_p$ are the collision and plasma wavelengths of metallic layer consecutively. For Au the ($\lambda_p$) and ($\lambda_c$) are about $1.6826 \times 10^{-7}$m and $8.9342 \times 10^{-6}$m respectively [16, 17]. Note that $\lambda_c$ in eq. 2 is for metal layer but in bulk case. If the metal layer consists of metal NPs it necessary to calculate a new $\lambda_c$. The finite size of the spherical NPs caused reduction in the free path of Drude electrons as well as the size based-damping constant of Drude electrons for metal is given by [18].

$$\epsilon_m = 1 - \frac{\lambda^2 \lambda_c}{\lambda_p^2 (\lambda_c + i\lambda)} \tag{2}$$

For bulk material $\Gamma_{\text{Bulk}}$ is the damping constant, $A$ is constant equivalent an amount near unity, $v_f$ is the Fermi velocity and $R$ is the radius of the spherical NP. The wavelength of bulk collision ($\lambda_{c_{\text{Bulk}}}$) conducted to the oscillations damping of electron density. In the reason of electrons collisions inside the bulk metal. For the bulk expression, a collision wavelength in equation (3) takes the final formula as mention below to provide the size-based of collision wavelength ($\lambda_c$),

$$\frac{c}{\lambda_c} = \frac{c}{\lambda_{c_{\text{Bulk}}}} + \frac{A v_f}{R} \tag{3}$$

In this paper, Au NPs are taken as spherical in shape with various radius of ($R$) 20 nm, 30 nm, 40 nm and 50 nm.

3rd Medium: sensing medium: is the chemical sample (target) in this research. Its dielectric constant is indicated by $\varepsilon_s$ ($\varepsilon_s = n_s^2$).

2.2. The resonance conditions

Now if a ray of polychromatic light guided into the optical fiber incident on the metal layer coated over the core then an excitation occurs in the surface plasmon wave. If the wave vector of the incident light equal to that of the plasmon wave, a resonance occurs. Hence the resonance condition can be written as:

$$\frac{2 \pi}{\lambda} n_1 \sin \theta = \text{Re}(K_{sp}) \tag{5}$$

Where $n_1$ is a core refractive index, $\theta$ is the incident angle on the metal-core interface, $\text{Re}(K_{sp})$ is a real part of the surface plasmon wave vector that can written as:

$$k_{sp} = \frac{\omega}{c} \sqrt{\frac{\varepsilon_m \varepsilon_s}{\varepsilon_m + \varepsilon_s}} = \frac{2 \pi}{\lambda} \sqrt{\frac{\varepsilon_m n_s^2}{\varepsilon_m + n_s^2}} \tag{6}$$

Where $\varepsilon_m$ and $\varepsilon_s$ are the metal dielectric constants and sensing area consecutively. $\omega$ is the incident wave frequency and $c$ is a speed of light.

2.3. Transmitted power

The formulation of the incident light reflection coefficient for (P-polarized) is gotten by implementing the matrix method of N-layer model [19]. Since the SPR phenomenon does not occur when the
incident ray has an S-polarization. The light power transmitted by the fiber can be under the best resonance conditions, only half of the power injected at the input face of the fiber. So that the final expression of $P_{trans}$ can be written in the following form:

$$P_{trans} = \frac{1}{2} \left[ \frac{\int_{\theta_{cr}}^{\frac{\pi}{2}} R_p N_{ref}(\theta) \left( \frac{n_1^2 \sin \theta \cos \theta}{1 - n_1^2 \cos^2 \theta} \right)^2 d\theta}{\int_{\theta_{cr}}^{\frac{\pi}{2}} \left( \frac{n_1^2 \sin \theta \cos \theta}{1 - n_1^2 \cos^2 \theta} \right)^2 d\theta} + 1 \right]$$

(7)

Where $N_{ref}(\theta)$ is the total reflections achieved through a beam making an angle $\theta$ with the normal to the core-metal layer interface in the sensing area that is given by [18]:

$$N_{ref}(\theta) = \frac{L}{D \tan \theta}$$

(8)

Where $L$ and $D$ are the sensing area length and the fiber core diameter respectively. The critical angle of the core-clad interface is given by [18]:

$$\theta_{cr} = \sin^{-1} \left( \frac{n_{cl}}{n_1} \right)$$

(9)

Where $n_{cl}, n_1$ are the refractive index of the clad and core of the optical fiber consecutively.

### 2.4. Sensitivity and Resolution

The sensitivity can be defined as alter in resonance wavelength per unit change in refractive index of the sensing medium and it can be expressed as [20]:

$$S_n = \frac{\Delta \lambda_{res}}{\Delta n_s}$$

(10)

Where $\Delta \lambda_{res}$ and $\Delta n$ are the change of the resonance wavelength and refractive index respectively. On the other hand, the capability to observe the smallest difference in the analyte is called the resolution. It can be calculated according the following equation [20]:

$$R = \frac{\Delta n_s}{\Delta \lambda_{res}} \Delta \lambda_{DR}$$

(11)

Where $\Delta \lambda_{DR}$ is the spectral resolution of the spectrometer.

### 3. Results and discussions

In this work, several different chemical liquids (water, Acetone, Ethanol, Acetic Acid, and Kerosene) that have refractive index of 1.330, 1.36, 1.361, 1.37, 1.39 respectively are supposed like sensing mediums. The measuring values of the parameters considered as follow: Fiber numerical aperture = 0.24, the fiber core diameter $D = 600 \mu m$, exposed sensing region length $L = 10 \text{ mm}$ and Au NPs layer total thickness steadied at 50nm. To study the effect of Au NPs size, different sizes 20, 30, 40, and 50nm were utilized. Fig.2 illustrates the curves of LSPR at different size of Au NPs for the studied chemical liquids. A dip occurs at a resonance wavelength. The enhancement of resonance wavelength with refractive index increment is related to the real part of the dielectric function of metal and then to the real part of propagation constant (Ksp). In addition, for large values of refractive index of the sensing area, the real part of the propagation constant of SPW will be higher and hence the resonance condition will satisfied at higher wavelength [19, 21, 22].
Figure 2: LSPR curves at different size of Au NPs for different chemical liquids.

Fig. 3 explains the full width at half maximum FWHM of LSPR Curves for the studied liquids at different sizes of Au NPs. The FWHM of each curve were reduced as a Au NPs size increased. To interpreted this effect in forms of fluctuation in light absorption as a result of the Au NPs particle size alteration [23]. When the imaginary part of $K_{sp}$ compatibles to the absorption of the incident light. In addition, intensity absorption of incident light considered for smaller particle size of Au NPs. Thus the intensity of transmitted light in the optical fiber was decreased and the SPR curve shifts going down. Consequently, the smaller the Au NPs particle size, the larger will be the dipped shifting. Hence enlarging of the SPR curve.

Figure 3: FWHM of LSPR Curves for different chemical liquids at different size of Au NPs.
Fig. 4 explains the sensitivity changing and resolution of LSPR-FO sensor with Au NPs particle size of 50nm at steadied thickness of Au layer. This is related to the light absorption alteration as a result to the Au NPs particle size variation [24].

![Figure 4: The Sensitivity and Resolution as a function of Au NP Size.](image)

4. Conclusion

A proposed (LSPR-FO) chemical sensor has been simulated and theoretically studied. LSPR curves for the sensor with different sizes of Au NPs and for different chemical liquids described clearly. Substances with high refractive indices showed high resonance wavelengths. The sensitivity and resolution have been evaluated for each size of Au NPs. The results exhibited increasing of resolution as the NPs size increase but the sensitivity reduced slightly. Nevertheless, sensitivity and resolution analysis have very benefit quantities can be used for similar systems. The N-layer modelling with the proposed matrix method provides a good simulation to the LSPR-FO sensor and evaluates its performance parameters. This study shows that the optimized LSPR-FO sensor has promising chemical sensing applications.

5. References

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