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Structure Design and Sensitivity Optimization of Optical Fiber Biosensor Based Au Nano Column - TiO_2 Heterostructure

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Abstract

An investigation on a single mode optical fiber sensor-based surface plasmon resonance was carried out in this work. A titanium dioxide (TiO_2) coated gold Nano-column (Au) are deposited on the proposed sensor and theoretically analyzed using COMSOL Muliphysics software 5.3. Presence of TiO_2 over the Au Nano-column can improve the sensitivity of the sensor and tune the resonance peak of transmission spectrum from visible region to near-infrared region. The size effect of TiO_2 nanoparticles on the sensor performance is studied. The optimum parameters of such as Au size and separation width between the Au Nano-column have been selected to enhance the performance of the sensor. In comparison, the sensor with TiO_2 over Au Nano-column is significantly improve the sensitivity and develop the sensor performance. The greater sensitivity of 5243.76 nm/RIU (refractive index unit) is obtained of sensor with TiO_2 over Au Nano-column when the external refractive index of analyte is varying from 1.33 to 1.39, while sensitivity of the sensor coated with Au Nano-column is obtained to be 4643.17 nm/RIU for the same analyte range. Above results can be used to predict the best parameters values of the sensor that corresponding to the greatest sensitivities of detection and finally opening new study in the field of gas sensors.

Keywords: Optica fiber sensors, SPR, Gas sensors, Bilayers

Introduction

In our communities, there is always need to improve of inexpensive sensors, stable sensors and measuring systems for services automation and micro-electronics with a brilliant performance. Attentions have been increased to study the model of the systems and structural survey of the materials for sensors improvement. In many forms, using optical fiber as a gas sensor is become more and more important [1-3]. Surface Plasmon Resonance (SPR) based optical fiber sensors is vital for the gas sensing. The work of SPR is based on the resonance phenomenon when the surface plasmon wave (SPW) is excited between the metal and dielectric material [4-7]. The main advantages of this technology is to characterize the properties of different materials such as molecular [8], biomolecular [9] and chemical interactions [10] in real time with no need to use the complex devices. The optical fibers for gas sensing are simple to use due to their advantages such as low cost and weight light [11]. These advantages were attracted the attentions of the researchers to combine the optical fibers with SPR technologies which are an effective solution as commercial sensors [12]. The collaboration between the SPR technology and optical fiber sensors have made a considerable progress, this collaboration is providing some additional advantages such as reduction, versatility and capability of remote sensing [13-15]. A commonly metal such as gold (Au), silver (Ag), copper (Cu), nickel (Ni) and aluminum (Al) are usually used in SPR based optical fiber sensors as they have a plenty of free charge carriers [16,17]. Amongst these materials, Au is usually used in SPR based optical fiber sensors due to its properties such as chemically stable and not oxidized. Additionally, Au possess absorption peak in the visible region [18-20]. However, the sensors require a robust material when exposed to the gas in the harsh environment. So, the metal oxides such as Titanium dioxide (TiO_2) could be a candidate material to detect the toxic substances due to its good properties such as high refractive index, highly light confinement, cost-effective, high stability and resistance to the corrosion and to the chemicals [21,22]. In addition, by using a conducting metal oxide such as TiO_2 with Au, the operating wavelength of the sensor based SPR moves to NIR area [23-26] owing to lower carrier concentration of TiO_2 (N'1020 cm^{-3}) comparing to the Au (N'1023 cm^{-3}). To evaluate the behavior of the fiber sensor, simulation methods are essential tools to analyze different parameters such as effective refractive index and the intensity. However, some drawbacks could be appearing through developing a good program of simulation. In particular, once the sensor construction is complex, the calculation is become very cumbersome and its need to long time. So, it is important to find a simple and non-complex method for analyzing parameters smoothly [27-30]. Different methods are used for modeling and simulation optical fiber sensors based SPR such as, expansion and propagation method [31], and multilayer structure transfer matrix modeling [32,33]. These methods are allowed a good estimate to the cylindrical structure, but their results are fail to describe the optical fibers structures in nano-scale. The finite difference time domain (FDTD) may be the solution which allows calculating the distribution of magnetic and electric field. However, it is required huge size of computing memory [34]. These obstacles are solved using the COMSOL Multiphysics software which is used to optimize the size of particles in nano scale with short time computing.

The aim of this work is to develop the sensitivity of the sensor and to enhance the accuracy of the single-mode optical fiber with TiO_2 over Au Nano-columns heterostructure using COMSOL Multiphysics software 5.3. The software is used for optimization the size of TiO_2 and Au in Nano columns, and to investigate the effect of TiO_2 diameter on sensitivity. The results illustrated that the sensor sensitivity can be significantly enhanced with presence the TiO_2 on the optical fiber structure.

Materials and methods

Heterostructure of semiconductor-metal

Heterostructure is the contact between a semiconductor and another material (liquid, gas, or metal), usually is involve the rearrangement of electric charges which are lead to form a double layer. The space charge layer is producing when the charge carriers are transfer between the semiconductor and the contact phase, and also it can be produced via charge carriers that trapped at the states of the interface. The generate defects in the semiconductor/conductor junction are play the main way to transfer the electron from one material to the other. The created Schottky barrier in the junction is impeding the charge carriers from return to the conduction band of the semiconductor. Usually, thin film of metal can be used to achieve the highest potential to trap the electron. Even when the effect of the electron trap is incapable to shift the absorption spectrum of the heterostructure toward the red wavelength region, some photocatalytic activity can be achieved via surface plasmon resonance phenomenam (SPR). Additionally, the plasmonic coating play a great role to enhance the sensing features of the sensors. Generally, different metals were deposited on the optical fiber to excite the surface plasmon resonance. Although there is an improvement in the performance of the sensor, the fiber that coated by these metals still operate in the visible light range, which make the sensors less useful with communication devices. However, the researchers found that a high dielectric layer deposited over the metal could be developed the sensors performance toward the red wavelength. They found that the deposited TiO_2 over the Au can modify the wavelength resonance of sensor near to the infrared range [35,36]. So, the heterostructure based TiO_2 over Au Nano column is a promising candidate which can be used as gas sensors.

Theory and modeling

There are 2 forms of light energy when is propagating within an optical fiber which are refracted light and evanescent waves. The react between light and the photocatalysts using evanescent waves is more efficiently than refracted light. Additionally, the optical fiber based SPR sensor generates surface plasmon waves (SPW) using evanescent wave to excite the free electrons on the surface of metal. The energy that carried by incident photons (k is a wave number in free space, k_x is the component in direction x-axis and θ_o is the incident angle) at the interface of metal/dielectric can be transferred to electrons by absorbing a part of light energy, and then the resonance absorption peak will form in the spectrum. **Figure 1** illustrates the system poses 3 superposed layers, which are dielectric medium (ε_0), metal (ε_m).

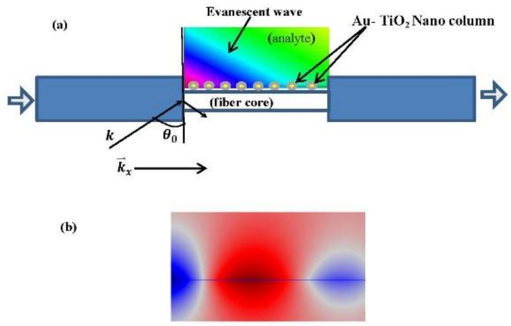

Figure 1 Schematic diagram of the detection-based SPR technique using COMSOL (a) surface plasmon polariton interface and (b) localized surface plasmon supported by a metal dielectric.

Figure 2 shows the graphic view of the designed optical fiber sensor coated with Au Nano columns - TiO_2 heterostructure. The magnification of the sensing length is shown in **Figure 2(b)**. Au Nano-columns are formed and arranged with the same diameter on the sensing length and then the Au coated with TiO_2. The intensity of electric field that induced at the interface between the metal-dielectric is dependent on the geometry of the particle [37,38]. This aspect is important for sensors to control the electric field by varying the shape, size and the inter separation of particles. In addition, when the distance gap between 2 Au Nano columns is large, the Au Nano-columns become non-interacting (isolated particles) [39,40]. However, if Au Nano-columns get a very close, individual plasmon oscillations from 1^{st} Au to 2^{nd} Au can be coupled by using their near-field interaction, which are resulting the coupled plasmon modes [41].

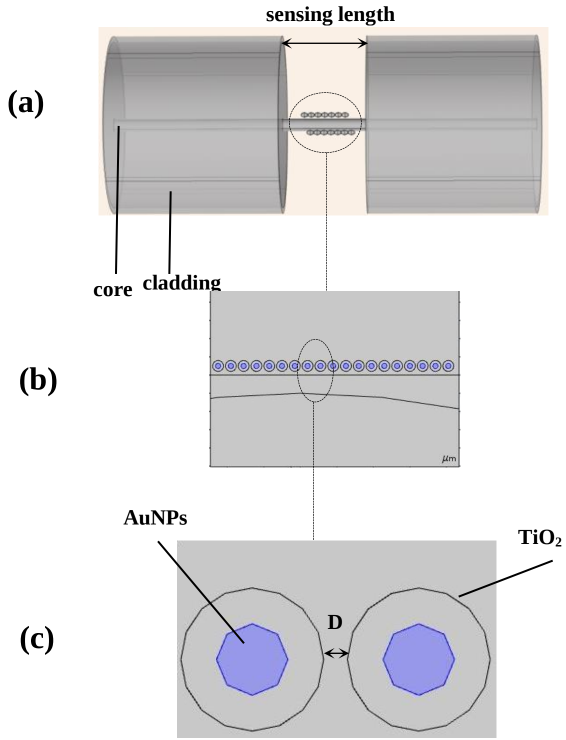

Figure 2 Graph of the designed optical fiber refractive index sensor (a) designed sensor coated with Au Nano column - TiO_2, (b) and (c) are the zoomed in of the Nano column covered the sensor.

The losses of optical fiber is calculated using the following formula:

$$\alpha = 2k_0 Im\,(n_{eff}) \tag{1}$$

where α, k_0 and $Im(n_{eff})$ are the attenuation constant, wave number in vacuum and the imaginary effective refractive index, respectively. The power of transmission light after coating the sensing length is calculated as following:

$$P_L = P_0 \exp(-\alpha L) \tag{2}$$

where P_0 and P_L are the input power of light and the output power after light passing through the sensor region, respectively.

The suggested sensor is considered using a typical single mode optical fiber with silica core (3.1 doped GeO2) and cladding (pure silica). The core and cladding diameter of 9 and 125 µm with refractive index of 1.4533 and 1.4504, respectively. The proposed optical fiber based SPR sensor (**Figure 2(a)**) is designed based on the etching method where whole cladding is removed. The sensing length (L) of 1 mm is used, and to maintain the integrity of the core thickness, the residual core is kept to 0.1 µm. Au Nano-column and TiO_2 are deposited onto the sensing length. The diameter of the Au Nano-column, diameter of the TiO_2 and the distance width between 2 successive Au Nano-columns are denoted by d_1, d_2 and D, respectively. In the meshing step, the 'extremely fine' is considered for Au and TiO_2 while 'finer' is selected for the entire structure. The Au Nano-column as the active metal is selected to stimulate surface plasmon at the sensing region due to its chemically stable in air. The permittivity (ε_m) of the Au is calculated using the Drude model as following:

$$\varepsilon_m(\lambda) = \varepsilon_{mr} + i\varepsilon_{mj} = 1 - \frac{\lambda^2 \lambda_c}{\lambda_p^2(\lambda_c + i\lambda)} \tag{3}$$

where, λ_p = 1.6826×10^{-7} m and λ_c = 8.9342×10^{-6} m are the plasma wavelength and the collision wavelength, respectively. The thickness of the Au Nano-column is set from 10 to 50 nm. The transmittance of light is calculated using the following equation:

$$T = \exp(-\frac{4\pi}{\lambda_o}\mathrm{Im}(\mathrm{n}_{eff})\mathrm{L}) \tag{4}$$

where, λ_0 is the incidence wavelength, $Im(n_{eff})$ is the imaginary part of the effective index, and L is the length of the sensing. The SPR response appears as a dip in the transition spectrum when the phase is matching between the surface plasmon mode and the fundamental mode of optical fiber. The TiO_2 thickness is varied from 5 to 30 nm to study its effect on the performance of the optical fiber based SPR sensors. The refractive index of the TiO_2 is calculated using the empirical relationship as following [42]:

$$n^2 = 5.913 + \frac{0.2441}{\lambda^2 - 0.08003} \tag{5}$$

The sensitivity of the optical fiber based SPR sensor can be represented as slope of the curve and it is expressed as:

$$s = \frac{\Delta\lambda}{\Delta n} \tag{6}$$

where Δn and $\Delta\lambda$ are the change in the external refractive index and the shifting in the corresponding resonant wavelength, respectively.

Results and discussion

Parameters optimization

In this work, Eqs. (3) - (5) have been used to calculate the refractive index of Au, the transmittance of light and the refractive index of TiO_2, respectively, to study the sensor performance. In addition, the size effect of TiO_2 nanoparticles on the optical fiber based SPR performance is studied. In the model, the diameter of the TiO_2 Nanoparticles changes from 4 to 30 nm with the step of 5 nm. Four layers (fiber core/Au/TiO_2/ analyte) of optical fiber structure based SPR sensor have been constructed and simulated using COMSOL Multiphysics Software 5.3. First of all, we optimized the surface coverage of Au Nano-column on the response of sensor. Different width between the Au (different surface coverage) are carefully chosen to find the best distance with good results. **Figure 3(a)** shows the transmission spectra versus wavelength as a width between Au Nano column varied from 5 to 40 nm with Au diameter of 40 nm and external refractive index of 1.33. It can be seen that as the distance of width increases from 5 to 20 nm, the transmission spectrum is become narrow with shifting toward longer wavelength. When the distance is larger than 20 nm, no shifting occurs in the spectrum. **Figure 3(b)** shows the sensitivity by plotting the position of the transmission peak versus the external refractive index (1.33 - 1.39). A linear regression is achieved and the slope of the fitted line is used to determine the sensitivity. It can be seen that the increasing in the distance between the Au does not influence the sensitivity of the sensor. Furthermore, when the surface coverage of the sensor region increases (Au Nano-column get close), the sensitivity of the sensor is increased due to coupled plasmon modes oscillations of each Au Nano-columns through their near field interaction. However, when the surface coverage of the sensor region decreases (the distance between Au Nano-column is large), the interaction between Au is gradually decrease, then the sensitivity also decreases. This result agrees with the behavior of Au metal as described in literature [39,44]. Based on the above results, the distance between Au Nano-column is choose to be 20 nm and this value is equal to half of the Au diameter.

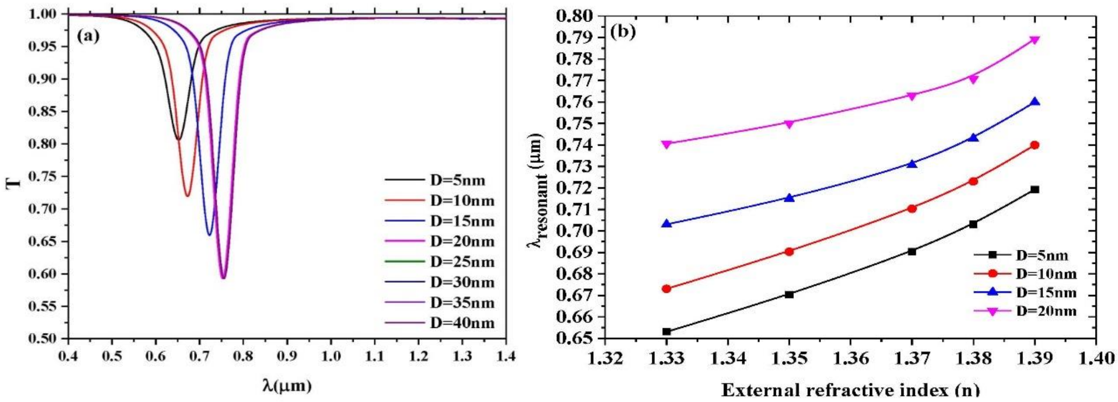

Figure 3 Optimization the width between Au Nano column (a) transmission spectra versus wavelength of different distance between Au Nano column (b) resonant wavelength with Au diameter of 40 nm and external refractive index = 1.33.

Figure 4 shows the sensitivity (S) in nm/RIU of the sensor verses the distance between Au Nano-column at the external refractive index of 1.33 and Au diameter of 40 nm. From **Figure 4**, it can be notice that the sensitivity increases linearly when the distance is increased, where the distance of 20 nm between Au produced the highest sensitivity. However, the sensitivity is kept constant when the distance is exceeded 20 nm due to decrease the interaction between Au. The maximum sensitivity is found to be 4531.54 nm/RIU.

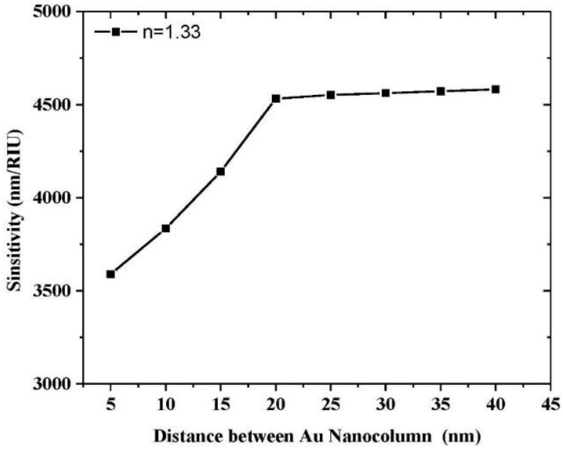

Figure 4 Sensitivity variation as a function of distance between Au Nano-column with Au diameter of 40 nm and external refractive index of 1.33.

Au Nano column-TiO_2 based SPR sensor

We optimized the diameter and the distance between Au Nano-column as d_1 = 40 nm and D = 20 nm, respectively. In the next structure, the TiO_2 is used to enhance the performance of the optical fiber sensors. The aim of this structure is to increase the interaction between the light and the external medium (increase the evanescent light). The TiO_2 is used as a dielectric material over the Au Nano-column. To exam the sensing ability of the suggested sensor, the loss is simulated for the external refractive index varied from 1.33 and 1.39. **Figure 5** shows the comparison SPR losses of the sensor with Au and the sensor with TiO_2 over Au when the diameters of Au and TiO_2 are 40 and 25 nm, respectively. It can be seen from **Figure 5** that the resonant wavelength moves to the longer wavelength (red shifts). We can say that the presence of TiO_2 over the Au Nano-column will increase the depth of evanescent wave. Consequently, the depth of electric field penetrating into the surrounding medium also increase, thus, improve the contact between the surface plasmon resonance and the external surrounding medium.

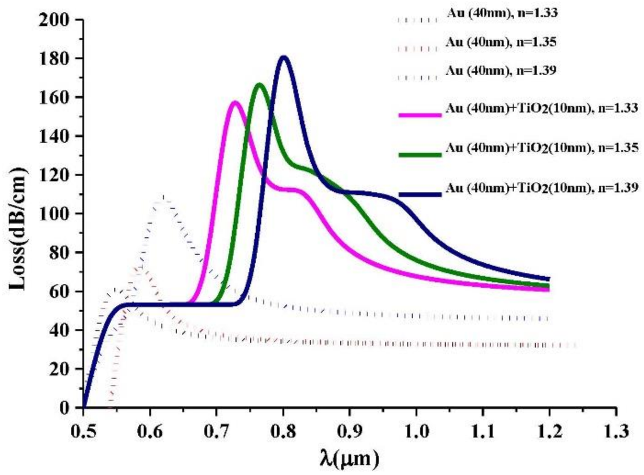

Figure 5 Loss as a function of wavelength for external refractive index of 1.33, 1.35 and 1.39, (dot line) for the sensor with Au Nano column, and (solid line) for the sensor with TiO_2 coated Au.

The enlarged view of the electric field distribution at n = 1.39 for sensor with Au and sensor with TiO_2 over Au are shown in **Figures 6(a)** and **6(c)**, respectively. **Figures 6(b)** and **6(d**) illustrates the normalized electric field intensity when exposed to external refractive index of 1.39 for the sensor with Au and sensor with TiO_2 coated Au, respectively. The enhancement in the sensitivity is confirmed by plotting the profiles of the normalized field along y-axis (Ey). Here, it can be observed that the peak of normalized field for sensor with TiO_2 coated Au (**Figure 7(c)**) is greater in comparison to sensor with Au (**Figure 7(d)**). This demonstrates that additional coupled energy from the core mode into the SPP modes of sensor with TiO_2 coated Au Nano column is higher, and here we can prove that the sensor become more sensitive to the external refractive index.

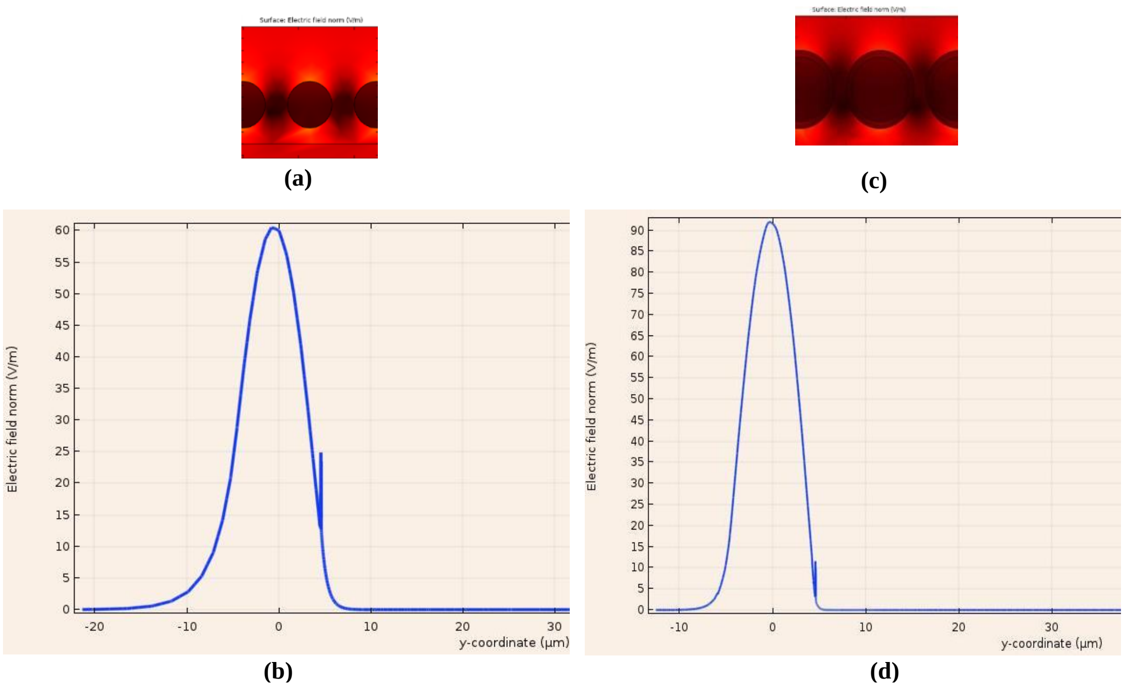

Figure 6 (a) and (c) The electric field distribution and (b) and (d) the normalized electric field for the sensor with Au and sensor with TiO_2 coated Au, respectively, the external refractive index is 1.39.

Figure 7 shows a strong resonant plasmon as a function of wavelength at different diameter of TiO_2 varied from 5 to 30 nm with external refractive index of 1.39. The transmission spectra is shifting from the visible regions (750 nm) to the near infrared regions (1066 nm) when the diameter of TiO_2 increased as illustrated in **Figure 7(a)**. **Figure 8(b)** illustrates the resonant wavelength as a function of the external refractive index at different diameter of TiO_2, the sensitivity of the SPR sensor is gradually increased when the refractive index is increased. Here, the work function of Au metal is higher than the TiO_2 semiconductor, so the electron passage from the semiconductor to the metal arises till the 2 Fermi levels are aligned and this electrical contact is formed a space charge layer and accordingly, increasing the sensitivity.

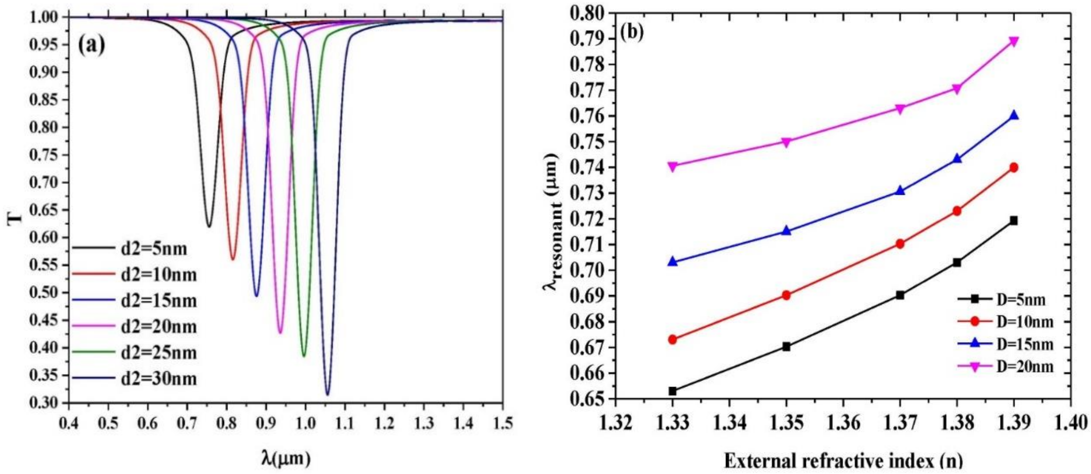

Figure 7 (a) Transmission spectra as a function of wavelength at different diameter of TiO_2 (b) of SPR resonance wavelength variation versus external refractive index different diameter of TiO_2 with Au diameter of 40 nm.

After parameters optimization, the sensitivity (S) in nm/RIU for sensor with TiO_2 over Au Nano-column illustrates in **Figure 8**. The optimum Au diameter is selected as 40 nm and TiO_2 diameter is varied from 5 to 30 nm, with external refractive index of 1.39 and distance width between the Au Nano-column of 20 nm. The maximum sensitivity at the refractive index of 1.39 is 5243.76 ± 0.074 nm/RIU. Here, the sensitivity has been increased about 15.7 % when the TiO_2 is coated the Au Nano-column compare to sensitivity of the sensor with Au Nano-column.

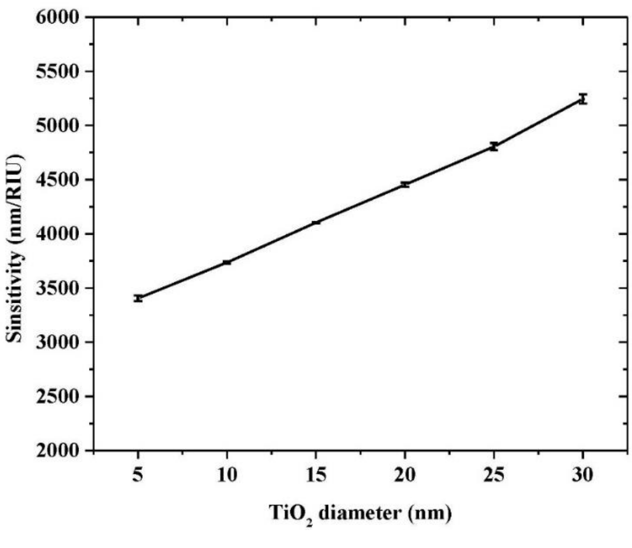

Figure 9 The sensitivity (S) of the sensor with TiO_2 coated Au Nano column.

At the analyte-TiO_2 interface, the evanescent wave and amplitude are greatly susceptible to change in the refractive index, this changes the signal of SPR and then enhance the surface plasmon which is in turn increases the detection accuracy. **Table 1** shows the comparison of sensitivities of the sensors with different thicknesses of Au Nano-column and TiO_2 at refractive index of 1.33, 1.35 and 1.39. In this paper and as can be seen from **Table 1**, the performance of the proposed optical fiber sensor is enhanced by using TiO_2 coated Au Nano-column.

Table 1 The comparison of sensitivities with different thicknesses of Au Nano column and TiO_2 at refractive indices (1.33, 1.35 and 1.39).

TiO_2 diameter (nm)		**Sensitivity (nm/RIU)**		**Au diameter (nm)**		**Sensitivity (nm/RIU)**	
External RI	n = 1.33	n = 1.35	n = 1.39	External RI	n = 1.33	n = 1.35	n = 1.39
5	1124.31	1351.16	3405.31	5	1687.57	1923.57	2117.68
10	1257.83	1483.26	3734.56	10	1910.72	2146.72	2296.38
15	1292.12	1511.65	4102.76	15	2221.64	2457.64	2605.31
20	1361.46	1689.36	4452.46	20	2423.27	2759.27	2934.56
25	1412.18	1754.97	4804.52	25	2584.96	2920.96	3202.76
30	1623.27	1983.15	5243.76	30	2747.46	3183.46	3652.46
				35	2860.47	3246.47	3984.52
				40	2926.84	3362.84	4531.54

Conclusions

The performance of the single mode-optical fiber sensors based SPR with TiO_2 coated Au Nano-column for refractive index measurement is studied and numerically analyzed. The optimization parameters and the sensing performance of designed sensor is investigated using FEM COMSOL Multiphysics 5.3. The TiO_2 is used in order to enhance the sensitivity of the designed sensor. The simulation results indicate that the sensitivity increased with increasing the TiO_2 diameter. The results show that the higher sensitivity of designed sensor can be reached to 5243.76 nm/RIU when the Au diameter is 40 nm, the TiO_2 diameter is 30 nm and the external refractive index of analyte is 1.39. Additionally, we found that the sensitivity is increased about 15.7 % compare to the sensitivity of the sensor coated with Au Nano-column. Hence, we can corroborate that TiO_2 over Au Nano-columns can significantly develop the sensitivity of the designed sensor. The above results display that the proposed sensor is capable to use in different chemical and gas sensing.

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