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Performance Evaluation of a Bilayer SPR-Based Fiber Optic RI Sensor With TiO_2 Using FDTD Solutions

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Abstract: We proposed a new bilayer surface plasmon resonance-based fiber-optic refractive index sensor with silver and an over-layer of TiO_2. We numerically investigated the optimal thickness of TiO_2 over-layer in the proposed sensor and compared its performance to that based on typical bimetallic layers of silver-and-gold in the aqueous media using finite-difference time domain approach. We show that the use of TiO_2 over-layer greatly improves the sensor performance in terms of sensitivity and signal-to-noise ratio compared to that with gold as the over-layer. Not only does the TiO_2 over-layer offer a cost-effective alternative to gold for overcoming the oxidation problem, but also it allows resonance wavelength-tunability.

Keywords: Bilayer, surface plasmon resonance (SPR), fiber optic sensor, refractive index (RI), finite-difference time domain (FDTD)

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1. Introduction

The choice of metals in surface plasmon resonance (SPR) sensors is critical because they must exhibit free electron behavior as described by the free electron model. Silver (Ag) and gold (Au) are widely utilized in SPR sensors thanks to their good response to changes in the surrounding dielectric environment compared to other noble metals. SPR sensors with a thin layer of Ag exhibit an improvement in the sensitivity and detection accuracy compared to those with Au [1]. This is because silver has the largest $|\varepsilon_r/\varepsilon_i|$ ratio, where ε_r and ε_i define the real and imaginary parts of the permittivity, which account for the reflection and absorption of light in the metal, respectively [1, 2]. However, several researchers prefer to use gold because of its chemical stability against oxidation [3, 4]. Zynio *et al.* proposed a new structure based on bimetallic layers of Ag and Au on the prism-based configuration where Au was utilized as the outer layer [5]. Not only does this structure exhibit a good sensitivity, which is comparable to those with Ag only, but it also offers protection

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against oxidation. In [1], the same bimetallic structure was applied on optical fibers for the fiber optic absorption sensor, and it was shown that Ag to Au thickness ratio must be as high as possible in order to achieve a good sensitivity.

Another alternative for the protection of the SPR metallic layer is oxides over-layers thanks to their low cost and good chemical stability [6, 7]. The addition of oxide over-layers of high refractive indices such as titanium dioxide (TiO_2) extends the local E-field intensity at the interface between the oxide over-layer and sensing medium. An increase in the E-field intensity results in an increase in the shift in the SPR wavelength with the change in the refractive index of the sensing medium which will improve the sensitivity [8]. Titanium dioxide has received much attention in sensing applications due to its chemical stability, high refractive index (RI), and elevated dielectric constant [9]. For example, the aluminum (Al)/TiO_2 film has been used in sensors based on doubly deposited uniform-waist tapers [8]. The thickness of Al and TiO_2 layers enabled tuning the resonance wavelength range of these sensors. Recently, the performance of a prism-based SPR RI sensor coated with copper (Cu)/TiO_2 was investigated theoretically and compared to that coated with Au film only in angular and wavelength interrogation [10]. The implementation of optical fiber based-SPR sensors using Cu and oxides bilayers was reported in [4].

In this paper, we propose and study the performance of a bilayer SPR-based fiber optic RI sensor with the TiO_2 coated Ag film on the unclad single mode fiber using FDTD solutions, a commercial software that implements the finite-difference rime domain (FDTD) technique. The performance of the proposed sensor is compared to that with bimetallic layers of Ag and Au.

2. Numerical analysis

The same bimetallic structure previously reported by Gupta *et al.* in [1] is applied on the single mode fiber (SMF)-based SPR RI sensor as shown in Fig. 1(a). An equivalent planar waveguide of a four-layer system is considered to substitute the SPR probe to simplify the calculations as shown in Fig. 1(b). We assume that all the involved media are homogeneous with flat and smooth interface boundaries. The four layers are defined as follows:

(1) Layer 1: Unclad SMF (fiber core) of pure silica core.

(2) Layer 2: Silver layer. The relative permittivity of Ag is described by the Drude-Lorentz model as [11]

$$\varepsilon(\omega)=\varepsilon_\infty-\frac{\omega_p^2}{\omega^2+\mathrm{i}\Gamma_p\omega}-\frac{f_1\omega_1^2}{\omega^2+\omega_1^2+\mathrm{i}\Gamma_1\omega} \tag{1}$$

where ω_p is the plasma frequency of the material, Γ_p is the damping or relaxation rate, ω is the frequency of interest, f_1 is the weighting factor, Γ_1 is the Lorentz damping rate, ω_1 is the Lorentz resonance width, and i is the complex number, $\mathrm{i}=\sqrt{-1}$. For this study, the default Ag (silver) - Johnson and Christy model for the permittivity of silver is adopted. It is numerically fitted with the experimental data extracted from [12] leading to the following values: ε_∞=3.7180, ω_p=9.2093 eV, Γ_p=0.0200 eV, ω_1=4.2840 eV, f_1=0.4242, and Γ_1=0.3430 eV.

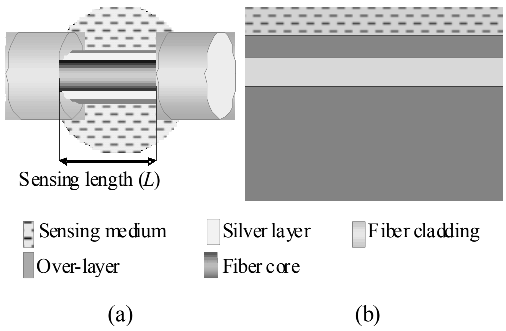


Fig. 1 Single mode fiber based SPR RI sensor's schematic diagram: (a) bilayer SPR-based fiber optic sensor and (b) equivalent four-layer waveguide planar structure.

(3) Layer 3: Over-layer. In the first configuration, gold is used as the outer layer. The properties of the gold layer are also calculated by (1), and the parameters are ε_∞ = 6.8890, ω_p = 8.9601 eV, Γ_p = 0.0723 eV, ω_1 = 2.9715 eV, f_1 = 1.7857, and Γ_1 =

0.9503 eV. In the second configuration, TiO_2 is utilized. The wavelength dependent RI of TiO_2 is represented by the following expression [13]:

$$n_3(\lambda) = \sqrt{5.913 + \frac{0.2441}{\lambda^2 - 0.0843}}. \quad (2)$$

(4) Layer 4: Sensing medium. The RI of the external medium is varied from 1.332 to 1.380 to observe the sensing capability of the proposed sensor in aqueous environment.

The resultant planar SPR structure was then modeled using FDTD solutions, which attempts to solve Maxwell's equations by using finite difference approximations to the spatial and temporal derivatives [14]. P-polarized light was guided into one of the fiber ends (in the forward *x*-axis direction) using a broadband light source with a wavelength ranging from 350 nm to 1700 nm, and the output power was recorded at the other end of the fiber. The *x* and *y* spans of the simulation region were set to 150 μm and 13 μm, representing the width and height of the structure, respectively. Perfectly matched layer (PML) boundary conditions for the sides and upper boundaries and an anti-symmetry boundary condition for the lower boundary were adopted to decrease the simulation volume and time by half. With the PML boundary condition, the incident light was absorbed without any reflection. Mesh refinement option was applied as the modeling used metal surfaces, and an auto non-uniform mesh with conformal variant 1 was selected to speed up the analysis. The SPR sensor response was plotted as the normalized transmitted power (i.e., to the source power) versus wavelength [15]. We observed the effect of the ratio of the Ag layer to the Au layer in the first configuration, and then we investigated the influence of a thin over-layer of TiO_2 on the sensor performance in the second configuration.

3. Results and discussion

Firstly, we numerically varied the thickness of the Ag layer using the theoretical model in Fig. 1 to find the optimum thickness. For this calculation, we ignored the over-layer. The optimized thickness that corresponded to the most pronounced dip at the resonance condition was found to be 60 nm. Figure 2 shows the SPR response curves for an SPR-based fiber optic RI sensor with a silver layer of thickness 60 nm over unclad fiber in two media. As seen from Fig. 2, silver exhibits very good response to changes in the RI of the surrounding environment, however, it is prone to oxidation. This problem can be mitigated by the use of an over-layer as follows.

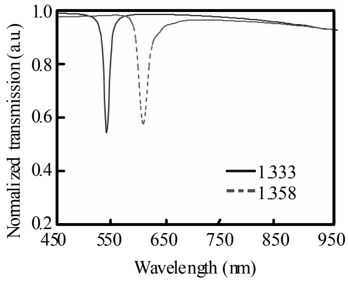


Fig. 2 SPR response curves using a single layer of silver in two different sensing media (RI=1.333 and 1.358).

In the first configuration, we used a constant total bi-metallic thickness of 60 nm. The silver-to-gold thickness ratio (Ag:Au) was varied as 1:0 (Ag only), 2:1, 1:1, 1:2, and 0:1 (Au only). The resultant SPR response curves within the aqueous medium (i.e., RI ~ 1.333) are plotted in Fig. 3. As seen from the figure, increasing Ag:Au thickness ratio makes the sensor performance more comparable to Ag-layer-only sensors.

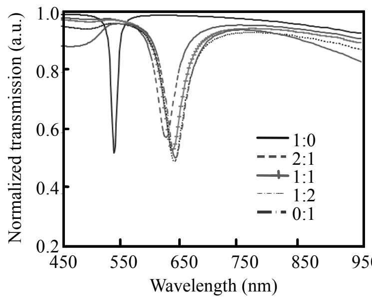


Fig. 3 SPR response curves using bimetallic Ag/Au configuration with various Ag:Au thickness ratios in the aqueous medium, i.e. RI is 1.333.

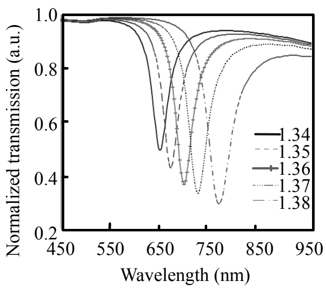
We performed additional simulations for a second medium with RI of 1.358 to investigate the effect of Ag:Au thickness ratio on the sensitivity and detection accuracy of the sensor. The sensitivity and signal to noise ratio (SNR) values were calculated from the plotted curves using (2) and (3) in [15] as shown in Table 1. The table illustrates that introducing a bimetallic layer instead of a single layer of gold improves both the sensitivity and detection accuracy of the sensor. Hence, we can choose a ratio that allows an excess of silver and thinner gold layer to protect the silver against oxidation.

Table 1 Sensitivity and SNR values for different bimetallic thicknesses of silver to gold for two different refractive indices, 1.333 and 1.358.

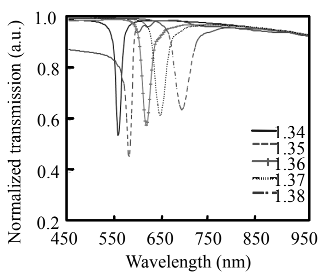
Ag:Au	$\Delta\lambda_{SPR}$ (nm)	$\Delta\lambda_{1/2}$ (nm)	S_n= $\Delta\lambda_{SPR}/\Delta n_s$ (nm/RIU*)	SNR= $\Delta\lambda_{SPR}/\Delta\lambda_{1/2}$
1:0	65	15	2600	4.33
2:1	55	33	2200	1.67
1:1	54	34	2160	1.59
1:2	53	39	2120	1.36
0:1	53	37	2120	1.43

*RIU=Refractive index unit.

From Fig. 3 and Table 1, 2:1 is found to be the optimum Ag:Au thickness ratio. The performance of the sensor in aqueous media was further investigated, and the results are depicted in Fig. 4. As seen from Fig. 4, the performance of the sensor is slightly degraded, especially in terms of SNR, when compared to the case of a single layer of Ag.



(a)



(b)

Fig. 4 SPR response curves using bimetallic Ag/Au configuration as the refractive index of the surrounding medium varies for a bimetallic Ag: Au thickness ratio of (a) 2:1 and (b) 1:0 (silver layer only).

To improve the performance, we proposed another configuration where we replaced the gold layer with a thin film of TiO_2. The thickness of the Ag layer (the active SPR layer) was maintained at the optimized value found earlier, i.e. 60 nm, whereas the thickness of the TiO_2 was varied from 15 nm to 30 nm to determine the optimal value. The resultant SPR response curves within the aqueous medium are plotted in Fig. 5. The figure shows that as the thickness of TiO_2 increases, the resonance wavelength is shifted towards the longer wavelength region, and the SPR curve is broadened.

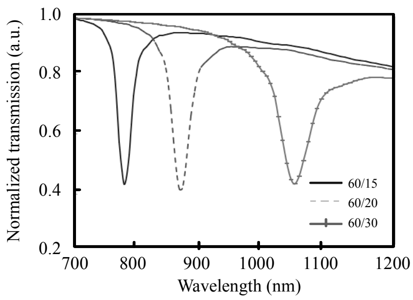


Fig. 5 SPR curves using the proposed Ag/TiO_2 configuration with different Ag/TiO_2 thicknesses ratios in the aqueous medium, i.e. RI is 1.333.

To investigate the effect of the TiO_2 layer thickness on the sensitivity and detection accuracy of the sensor, the additional simulation for a second medium with RI of 1.358 was performed. The sensitivity and SNR values are calculated from the plotted curves using (2) and (3) in [15] and summarized in Table 2. It is worth noting that the shift in the resonance wavelength is much more pronounced in the case of Ag/TiO_2 sensors compared to that of the Ag-layer-only sensors (Fig. 2), and it increases dramatically with the thickness of the TiO_2 layer which would boost up the sensitivity.

Table 2 Sensitivity and SNR values for different thicknesses of TiO_2 over-layer for two different refractive indices, 1.333 and 1.358.

Ag/TiO_2	$\Delta\lambda_{SPR}$ (nm)	$\Delta\lambda_{1/2}$ (nm)	S_n= $\Delta\lambda_{SPR}/\Delta n_s$ (nm/RIU)	SNR= $\Delta\lambda_{SPR}/\Delta\lambda_{1/2}$
60/15	95	22	3800	4.3
60/20	112	40	4480	2.8
60/30	160	80	6400	2.0

It should also be noted that as the TiO_2 layer thickness increases, the SPR curve width increases leading to the lower detection accuracy. Thus, by choosing a proper thickness for the TiO_2 over-layer, we can tune the resonance wavelength and improve the sensor performance. However, the broadening of the SPR curve must also be taken into consideration when choosing the TiO_2 layer thickness. For example, when the TiO_2 thickness is as high as 30 nm, the resonance dip becomes shallower and wider. Thus, the detection accuracy becomes very poor especially at higher refractive indices as shown in Fig. 6.

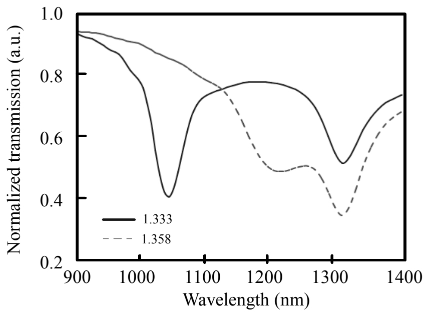


Fig. 6 Variation of normalized transmitted power with the wavelength when the thicknesses of silver layer and TiO_2 are 60 nm and 30 nm for two different sensing media, respectively.

The optimized thickness of the TiO_2 layer for sensing in aqueous environments was found to be 15 nm. The SPR response curves when RI was varied from 1.34 to 1.38 are shown in Fig. 7. The performance of the proposed Ag/TiO_2 bimetallic sensor in terms of the resonance wavelength as a function of the RI was compared to that using both Ag-layer-only and Ag/Au bimetallic configurations. The results are plotted in Fig. 8 which shows that replacing the gold with TiO_2 improves the sensitivity and SNR by factors of 1.70 and 2.6, respectively. Furthermore, a proper choice of Ag/TiO_2 bilayer system thickness (i.e. 60/15) can increase the sensitivity of the sensor by a factor of 1.5 while maintaining a detection accuracy comparable to that of Ag-layer-only sensors. This configuration can also be used when shifting the resonance wavelengths toward a specific spectral region is needed.

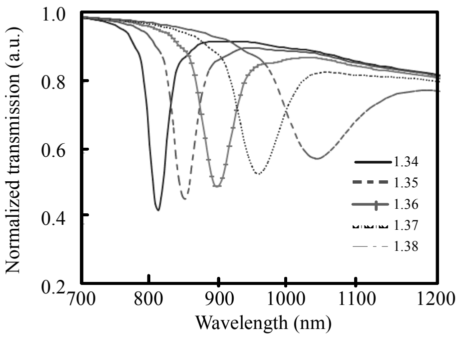


Fig. 7 Spectral response of the SPR-based fiber optic sensor with a 60-nm silver layer and a 15-nm TiO_2 over-layer for refractive indices ranging from 1.34 to 1.38.

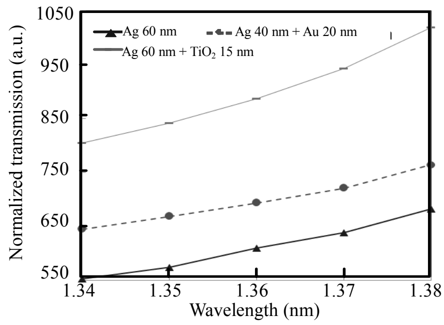


Fig. 8 Variation of shift in the resonance wavelength with RI for three different configurations.

4. Conclusions

We have proposed a new bilayer SPR-based fiber optic refractive index sensor with the TiO_2-coated Ag film and compared its performance with that of bimetallic layers of Ag and Au using FDTD solutions, a commercial software that implements the FDTD technique. We show that a bimetallic structure of silver and gold as the outer layer can protect silver from oxidation on the expense of a slight performance degradation compared to the case of Ag-layer-only sensors. However, replacing the gold layer with a thin film of TiO_2 (i.e. 15 nm) greatly improves the sensor performance in terms of the sensitivity and SNR by a factor of 1.70 and 2.6, respectively, compared to that with gold as the outer layer. In addition to being non-toxic, chemically stable, and relatively inexpensive choice, adopting the TiO_2 over-layer also allows tuning the resonance wavelength of the SPR sensor, which can broaden its range of applications.

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