Proposal of a plasmonic sensor based on 2D material $Ti_3C_2T_x$ MXene in terahertz frequency

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Abstract

In this paper, a plasmonic sensor utilizing bimetallic layer of Ag/Au with 2D material WS_2, and $Ti_3C_2T_x$ MXene is studied. The proposed SPR sensor is a free space structure using the Kretschmann configuration to stimulate surface plasmons (SPs). The finite-difference time-domain method is used to analyze the optical behavior of the proposed SPR sensor. The results show the proposed SPR sensor has the maximum sensitivity of 242 deg/RIU with 35 nm of Ag, 15 nm of Au with monolayer of 2D material WS_2 and one layer of $Ti_3C_2T_x$ MXene. We predict that the proposed structure can be used for biosensing and chemical sensing applications.

Keywords: Sensitivity, surface plasmon resonance, refractive index, sensor, $Ti_3C_2T_x$ MXene.

Introduction

Surface plasmon resonance (SPR) phenomenon is the resonant coupling of electromagnetic waves to the charge density oscillations at the interface of dielectrics and metals [1-3]. Due to the mismatch of optical momentum between the SPR mode and light in free space, the optical excitations in the SPR occur with the attenuated total reflection (ATR) method, which was proposed by Kretschmann [1] and Otto [2]. There is only a TM polarized electric field for surface plasmon waves (SPWs), this waves are exponentially decayed at the interface between the dielectric and the metal [4-7]. Surface plasmon resonance sensors have potential advantages such as real-time and label-free detections, high sensitivity, high-resolution detection, etc., which has led to their diverse applications [8, 9]. Various applications of SPR sensors include environment monitoring, medical diagnostics such as detection of human blood group, DNA, glucose, virus, living cell analysis, gas sensing, and so on [10- 12]. The 2D materials have desirable physical and structural properties and are well-suited for applications in sensing and biosensing. This is due to great adsorption surface area, direct bandgap, unique optical, chemical, thermal, magnetic, and electrical properties [13-15]. Transition-metal carbides and nitrides, known as MXenes, are 2D-materials by the general formula $M_{n+1}X_nT_x$, where M represents an early transition metal, X is carbon and/or nitrogen, and T_x is the surface termination groups ((–O), (–F), and (–OH)) [3, 16-19]. The index n indicates a variable number between 1 and 3. Among the types of MXene, $Ti_3C_2T_X$ MXene has shown potential in numerous fields, and due to its unique optical and electrical properties improves sensor performance and quality [3, 19, 20]. In recent years, the various structures of plasmonic sensors have been studied to improve the performance parameters of sensors, especially sensitivity [3- 5, 10, 15, 16]. In this work, we presented a plasmonic sensor based on the BK7 prism, silver/gold (Ag/Au) bimetallic films, 2D materials tungsten disulfide (WS_2), and MXene ($Ti_3C_2T_x$) under angular interrogation technique. The proposed sensor is a free space structure using the Kretschmann configuration to stimulate SPs. The performance parameters of the SPR sensor are investigated using the numerical method of finite-difference time-domain (FDTD) in the terahertz frequency.

Sensor Structural Configuration

The schematic of the proposed SPR sensor based on the Kretschmann structure is illustrated in figure 1. The structure consists of six layers, including BK7 prism, silver/gold (Ag/Au) bimetallic films, tungsten disulfide (WS_2), and MXene ($Ti_3C_2T_x$), and sensing medium.

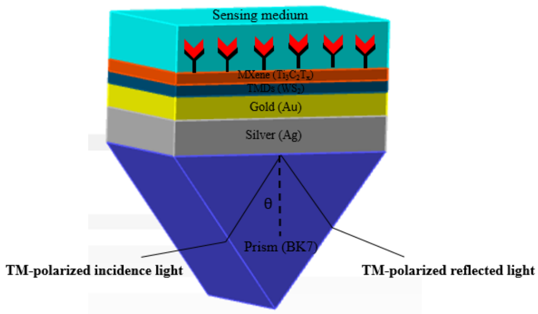


Figure 1. Schematic diagram of the proposed SPR sensor.

The finite-difference time-domain technique is used to evaluate electromagnetic field analysis for the proposed sensor. The parameter sweep is used for angular interrogation over a wide range of source angles (40° to 85°), in order to obtain the source angle capable to excite the SPR mode. The optical parameter was set as a plane-wave source (Bloch/periodic type) at an optical wavelength of 633 nm. Further, the perfectly matched layer (PML) profile was set to steep angle to be used as boundary condition for calculating the complex propagation constant of the modes. Also, for excitation of the SPW, the incident light is a transverse magnetic (TM) polarized. In proposed sensor, we use BK7 prism with n_{BK7}= 1.5151 at λ= 633 nm as the coupling prism for exciting SPR [3, 4, 16]. According to the Drude–Lorentz model, the refractive indexes of the metals are determined by [3, 4, 15, 16]:

$$n_m(\lambda)=\sqrt{\left[1-\frac{\lambda^2\lambda_C}{\lambda_P^2(\lambda_C+i\lambda)}\right]} \quad (1)$$

where λ_p and λ_c represent the plasma and collision wavelength. These two parameters for gold and silver are given in Table 1 [3, 4, 15, 16]. To reduce the oxidation of the Ag layer, the Au film is deposited on the Ag layer. Furthermore the use of a bimetallic structure enhances sensitivity in the SPR sensor highly. The complex RI of tungsten disulfide (WS_2) is $n_{WS_2} = 4.89 + 0.314\,i$, and its thickness is equal to 0.8 nm [3, 4, 15, 16]. The complex RI of $Ti_3C_2T_x$ MXene is $n_{MXene} = 2.38 + 1.33i$, and its thickness is equal to 0.993 nm [3, 4, 15, 16]. The last layer is the sensing medium and the RI of this medium is given as n_s= 1.33 + Δn_s, where Δn_s is the change of RI in sensing medium due to the occurrence of a biological action. This varies from 1.33 to 1.35 when biomolecules are adsorbed at the MXene sensing layer surface.

Table 1. The plasma and collision wavelength for silver (Ag) and gold (Au) [3, 4, 15, 16].

Metal	λp (m)	λc (m)
Ag	1.4541×10^{-7} m	1.7614×10^{-5} m
Au	1.4541×10^{-7} m	1.7614×10^{-5} m

Performance Evaluation Formula

The following performance parameters defined for the plasmonic sensor are sensitivity, DA, FWHM, and FOM. The sensitivity defined as the ratio of SPR angle shift ($\Delta\theta_{SPR}$) to changes in the refractive index (Δn_s) in the sensing medium by the following equation [17- 19]:

$$S=\frac{\Delta\theta_{SPP}}{\Delta n_s}\left(\frac{\deg}{RIU}\right) \quad (2)$$

The figure of merit (FOM) is obtained from the ratio of the sensitivity to the FWHM based on equation (3) [17-19]:

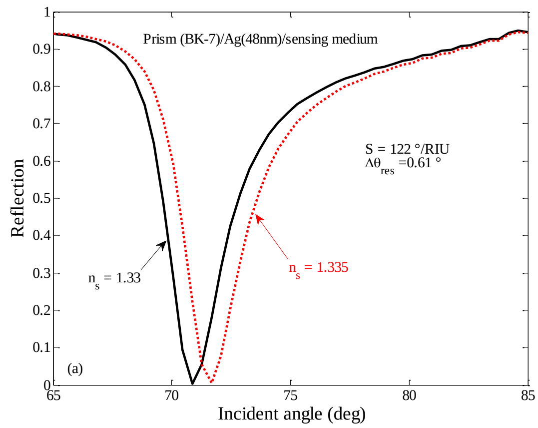
$$FOM=\frac{S}{FWHM}(RIU^{-1}) \quad (3)$$

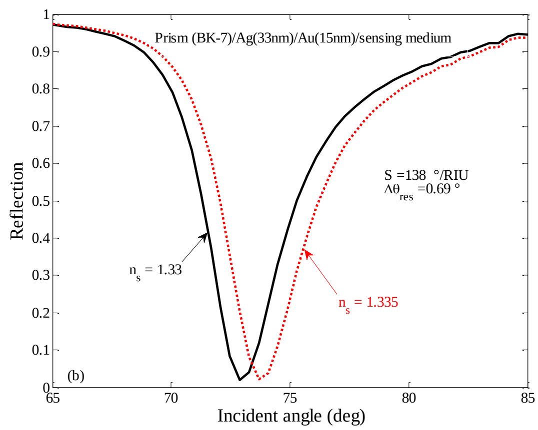
where full width at half maximum (FWHM) is a difference of the resonance angles at 50% reflection intensity [17-19]. FWHM also shows the angular width of the reflectance curve. Another critical parameter of SPR sensor is the detection accuracy (DA) can be determined taking the inverse of the FWHM of the SPR curve by using the following equation [17-19]:

$$DA=\frac{1}{FWHM}(\deg^{-1}) \quad (4)$$

Results and Discussion

We describe the role of each of the layered used in the proposed structure via the SPR curve. SPR characteristic curves for four structures include: structure 1- BK7 prism/Ag/ sensing medium, structure 2- BK7 prism/ Ag/ Au/ sensing medium, structure 3- BK7 prism/ Ag/ Au/ WS_2/ sensing medium, and structure 4- BK7 prism/Ag/Au/WS_2/ $Ti_3C_2T_x$ MXene/ sensing medium are presented in figure 2(a)–(d) respectively. The inset curvs within figure 2(a)–(d) show the variation of reflection with RI of the sensing medium for 1.33 and 1.335, on the adsorption of biomolecules on the sensor surface. We calculate resonance angle shift for the sensing layer RI variation of (Δn_s = 0.005) for four structures. Resonance angle shift obtained from SPR curves shown in figure 2(a)–(d) for structure1, 2, 3 and 4 are 0.61°,0.69°, 0.81°,and 1.21° respectively. Sensitivity calculated from above resonance angle shift for mentioned stuctures are 122 deg/RIU, 138 deg/RIU, 162 deg/RIU, and 242 deg/RIU respectively. Based on the results, it can be found that the introduction of $Ti_3C_2T_x$ MXene in the plasmonic sensor contributes to sensitivity enhancement. This is due to strong charge transfer between $Ti_3C_2T_x$ MXene /WS_2 layer and bimetallic Ag/Au layers





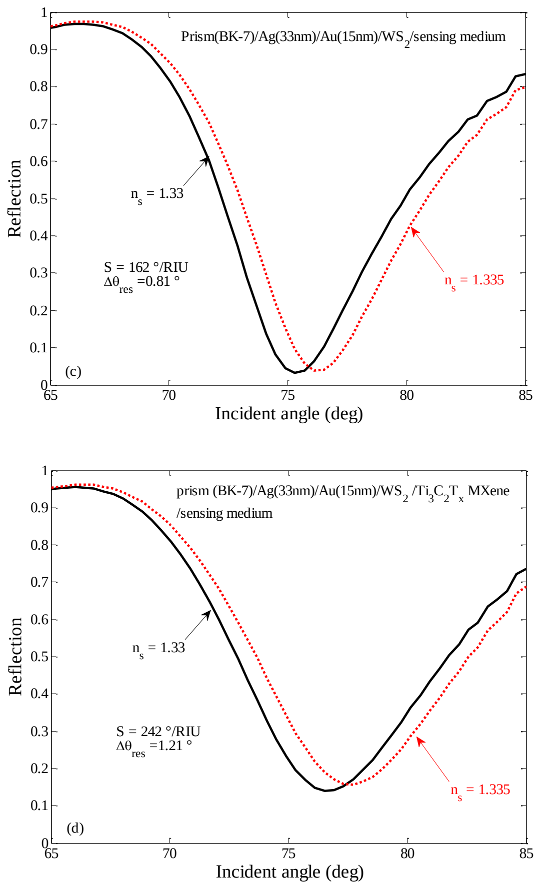


Figure. 2. The reflection as a function of the incident angle for (a) Structure 1, (b) Structure 2 (c) Structure 3 and (d) the proposed SPR sensor (Structure 4).

Figure 3 shows the absorption curve variation with the RI of sensing layer. As can be seen, by increasing the RI of sensing layer the plasmon resonance occurs at a larger angle. We have considered the SPR angle obtained for different RI values of sensing layer from n_s = 1.33 to 1.35 for the step of 0.005 of the sensing medium.

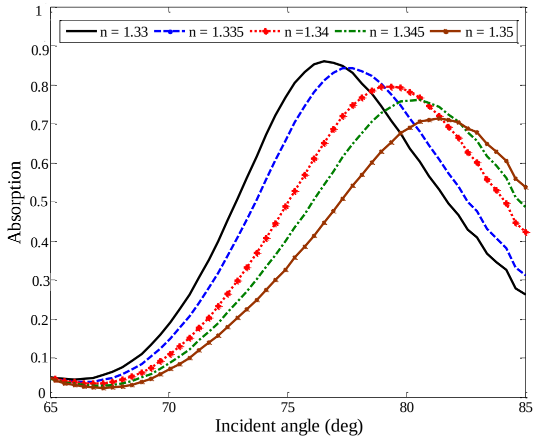


Figure. 3. The absorption curve as a function of the incident angle for proposed structure.

Figure. 4 plots the performance parameters variation with sensing layer RI. It can be seen that the sensitivity, minimum reflection, DA, and FOM of proposed SPR sensor varies from [242 to 287 deg/RIU], [0.1566 to 0.2854], [0.116 to 0.112 deg^{-1}], [28.07 to 32.43 RIU^{-1}] respectively, for the RI variation of sensing layer from 1.33 to 1.35.

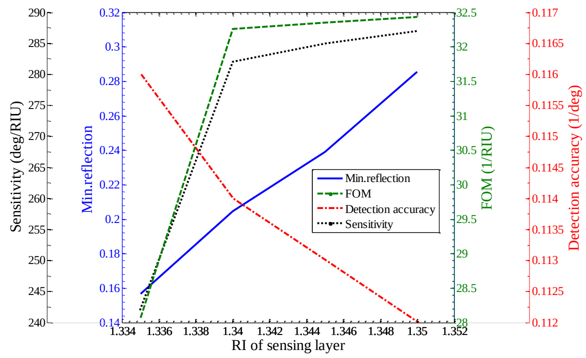


Figure. 4. Performance parameters variation with the RI of sensing layer for proposed SPR sensor.

Table 2 illustrates the comparison between the proposed SPR sensor with recently plasmonic sensors explored by different research groups. The proposed structure shows the highest sensitivity compared to the other structures at 633 nm. We expect that such promising results will lead the proposed structure as a potential candidate for detecting biomolecules and other analytes and can be used for biosensing and chemical sensing applications.

Table 2. Comparison of the Sensitivity of the proposed sensor to other existing plasmonic sensors.

Structure	Sensitivity (deg/RIU)	λ(nm)	Ref
BK7/Ag/Si/MXene	231	633	[15]
BK7/Si/MoS_2/ graphene	210	633	[18]
BK7/Au/WSe_2/Graphene	178.87	632.8	[19]
BK7/Au/BlueP-MoS_2/Antimonene	194.8	633	[20]
This work	242	633	-

Conclusions

In this paper, a plasmonic sensor including BK7 prism, bimetallic layer of Ag/Au, 2D material WS_2, $Ti_3C_2T_x$ MXene and the sensing medium introduced. The FDTD method was used to analyze the performance of the SPR sensor. The results show the proposed SPR sensor significantly improves sensitivity. The highest sensitivity of 242 deg/ RIU can achieve using Ag with a thickness of 35 nm, Au with a thickness of 15 nm, monolayer of WS_2 and $Ti_3C_2T_x$ MXene. The proposed sensor potentially opens a new possibility for the biological detection and other analytes.

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