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2D Nanomaterial-Based Hybrid Structured (Au-WSe₂-PtSe₂-BP) Surface Plasmon Resonance (SPR) Sensor With Improved Performance

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ABSTRACT As a promising optical method used in a variety of applications surface plasmon resonance (SPR) sensors are employed over a wide range of boundaries. This research proposes a highly sensitive SPR based sensor with a novel hybrid structure using transition metal dichalcogenides (e.g. WSe₂, PtSe₂) along with black phosphorene (BP) through comprehensive numerical study. To analyze and evaluate the performances of the proposed sensor, the widely used transfer matrix method (TMM) was used. The performances of the sensor were measured in terms of reflectivity, sensitivity, detection accuracy (DA), and figure of merit (FOM). The sensor structure was optimized by changing different structural parameters of the hybrid architecture to obtain better performances. The results revealed that insertion of PtSe₂ with WSe₂ and BP over a gold layer of the conventional structure improved the performance of the sensor and the maximum sensitivity of the sensor was measured as 200 deg/RIU with a FOM of 17.70 RIU⁻¹. As well, the light penetration through the optimized sensor is investigated using the finite element method (FEM) based software. With this kind of high sensing capabilities, it may be convinced that the proposed sensor can be applied in different fields of biosensing to detect liquid biological and biochemical samples or analytes.

INDEX TERMS Surface plasmon resonance (SPR), transition metal dichalcogenides (TMDCs), sensitivity, finite element method (FEM).

I. INTRODUCTION

Nowadays, as a highly promising optical technique different structures based surface plasmon resonance (SPR) have been reported to be used in the detection of samples for chemical, biochemical, biological, environmental, and medical applications. In addition, due to rapid response and high sensitivity, SPR based sensors serve as one of the most effective sensors for bio-molecular sample identification. The sensors avoid

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the time-swallowing labeling process for molecular binding and provide real-time monitoring and analyzing capability of analytes of the sensing medium [1], [2]. Various optical techniques, such as sensors based on Raman scattering [3], planar waveguide [4], prism coupler [5], grating coupler [6], and optical fiber [7], have been reported as of now for the sensing applications. The basic working process of the optical sensors is the assessment of variation in the input incident light and finding out the changes in its properties at the output terminal. To be explicit, at the output terminal of the sensor, the variation in frequency, amplitude, phase,

wavelength, or polarization of light is measured and recorded. The technique often used in the prism coupled optical sensor is interrogation of incident light angle to detect the analyte or sensing medium refractive index (RI). Since SPR-based sensors are used to detect a very small difference in the sensing medium RI, thus the sensor should have very good performance characteristics. Sensitivity, Full width at half maxima (FWHM), detection accuracy (DA), and figure of merits (FOM) are the key performance parameters of the prism coupled optical sensor to measure the quality [8].

In Kretschmann configuration based SPR sensors, the plasmonic material is the utmost diametrical parameter to determine the characteristics of the sensors. Materials with an ample number of free electrons in their valance bands are usually considered as plasmonic components. Among all the plasmonic materials silver (Ag) and gold (Au) are considered ideal candidates due to their attractive characteristics. Ag is a strong candidate as it has excellent optical properties, like no interband transfer at the visible light frequency, small optical damping with sharper resonance dip. For enhancing the sensitivity of the SPR sensors, Ag material can be used, but poor chemical stability is shown by it. On the contrary, the Au film is superfluous chemically static comparing with the Ag film, potentially adherence along with the glass, and no reaction is delivered by it along inorganic ions [9]. In this proposed sensor, Au film is utilized as the plasmonic metallic layer coated on the BK7 prism substrate.

While Biacore first developed and released prism-coupled sensing devices on the market in 1990, academicians, analysts, and researchers are constantly working to further improve the characteristics of these sensors [10]. In recent years, despite traditional structures, hybrid structures of SPR sensors have become very prominent for improving the quality of the sensor. Also, two-dimensional (2D) nanomaterials have taken extraordinary consideration for the last decade owing to the unprecedented optical, electronic, and catalytic features [11]. Single-layer PtSe₂ has a similar forming pattern to graphene, but it also has excellent optical and electrical properties that are taken into great consideration as a 2D product beyond the ancestor members [12]. It has intrinsic quantum confinement effect and potential interlayer interaction with profoundly harmonic band gap. It also prompts a semimetal-to-semiconductor transition while moving from bulk to few-layer form and shows the biggest band gap of ~1.2 eV for monolayer PtSe₂ [13], [14]. PtSe₂ with plasmonic materials were studied to design SPR based sensors by Jia and co-workers [15]. Their study shows that applying PtSe₂ over Ag and Au can improve the sensitivity of the sensor up to 162 deg/RIU and 165 deg/RIU, respectively. Furthermore, some hybrid configurations using multiple 2D materials like WS₂-graphene [16], MoS₂-WS₂-WSe₂ [17] have been proposed for improving performance of the sensor. Li *et al.* [18] presented black phosphorene (BP) as a strong competitor to graphene with its excellent opto-electric properties, high carrier mobility and direct bandgap [19]. Recently, a new hybrid structure with 10 layers of BP

and monolayer of WS₂ have been considered to enhance the sensing performance in an Au based SPR sensor [20]. The proposed sensor showed the maximum sensitivity up to 187 deg/RIU. Thus, in addition to traditional architectures, hybrid SPR sensor designs using 2D nanomaterials have recently been presented as a way to improve sensor performance.

SPR is now extensively used in sensing a widespread area of physical, chemical, and biochemical parameters, including enzyme detection, food safety, wireless sensing applications, DNA–DNA hybridization, protein–protein, protein–DNA, early cancer cell detection, glucose detection, gas sensing and so forth [21]–[26]. To identify the samples, all SPR sensing techniques monitor the resonance points that are correlated to the change in refractive index (RI) of the sensing medium resulted from biomolecular interaction. In this paper, after analyzing different configurations of SPR based RI sensors, a new SPR sensor with hybrid structure is proposed using a heterostructure of black phosphorene (BP), PtSe₂, and WSe₂. The geometrical parameters of the sensor have been optimized using the trial and error method and the performances are numerically analyzed using the widely used transfer matrix method (TMM). Finally, the finite element method (FEM) based software is used to assess light penetration through the proposed sensor.

II. THEORETICAL MODELLING OF SPR SENSOR

The most accepted light coupling technique used for the excitation of surface plasmons (SPs) in SPR-based instruments is prism coupling. This light coupling is carried out with two configurations in SPR technology, and they are Kretschmann - Reather configuration [5] and Otto configuration [27]. Both configurations operate based on the concept of attenuated total reflectance (ATR). Kretschmann's configuration is used as the most common approach [5] in the SPR technique for its superior efficiency and ease of operation and manufacturing. In this paper, the raised SPR sensor structure is proposed based on Kretschmann's configuration as shown in Fig. 1.

Coupling light with lower-refractive-index prisms, such as CaF₂, reduce detection range and higher-refractive-index couplers reduce resonance dip of the sensor. A BK7 glass prism is used as a coupling system amidst this study because of its high efficiency and low refractive index (RI), which makes it suitable for pairing monochromatic plane-polarized light generated by a He-Ne laser with a wavelength of 633 nm [5]. Because of its superior sensing performances, such as better sensitivity characteristics, the Au film with a thickness of 50 nm was chosen as a plasmonic material [5]. The RI of the BK7 glass prism can be determined utilizing equation 1 [28]:

$$n_{BK7} = \sqrt{1 + \frac{1.03961212\lambda^2}{\lambda^2 - 0.00600069867} + \frac{1.01046945\lambda^2}{\lambda^2 - 103.560653} + \frac{0.231792344\lambda^2}{\lambda^2 - 0.0200179144}} \quad (1)$$

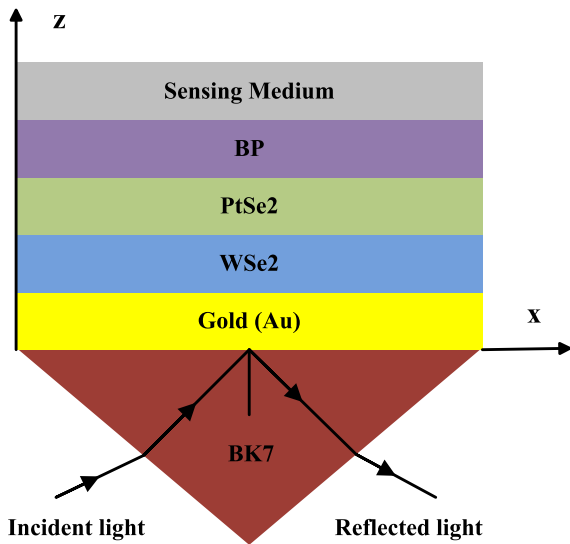


FIGURE 1. Two-dimensional (2D) illustration of the proposed hybrid structured SPR sensor.

where, λ stands for the wavelength of incident light. The RI of Au metal is determined using the wavelength-dependent Drude-Lorentz model [29]:

$$n_{metal}(\lambda) = \left(1 - \frac{\lambda \times \lambda_c}{\lambda_p^2(\lambda_c + i\lambda)}\right)^{\frac{1}{2}} \quad (2)$$

where λ_c stands for collision and λ_p stands for plasma wavelengths. The values of collision and plasma wavelength for Au are 8.9342×10^{-6} m and 1.6826×10^{-7} m, respectively.

The RI of BK7 glass is determined as 1.5151 at the wavelength of 633 nm, according to the equation 1. The heterostructure of PtSe₂ with 2D materials (e.g. WSe₂, BP) which is directly linked to the sensing medium or analyte is known as the affinity layer. It improves the sensitivity of the raised sensor and also eliminates the possibility of oxidation. The optical characteristics of PtSe₂ change with the thickness and experimental modulation are utilized for determining the complex RI of PtSe₂. At 633nm wavelength, the complex refractive indices of refraction are calculated as like $2.9189 + 0.9592i$, $2.8650 + 1.1867i$, and $3.02 + 1.4967i$, gradually for 2nm, 3.6nm, 4.4 nm of thickness [15]. The RI of WSe₂ is determined as $\eta WSe_2 = 4.55 + 0.4332i$, and the thickness of it is altered like $dWSe_2 = 0.70 \times p$ nm, whither p represents the extent of the WSe₂ layer [24]. Also, the RI of BP is calculated as $\eta BP = 3.5 + 0.01i$, and the thickness of BP is modulated as $dBP = 0.53 \times q$ nm, where q is the number of BP layers [20]. The RI of the sensing medium is calculated as $n = 1.33 + \Delta n$, where Δn refers to the RI alteration in the sensing medium due to biological activity or chemical reaction.

The sensor works based on the principle of attenuated total reflectance (ATR) in association with the angular interrogation technique. The ATR technique utilizes an attribute

of total internal reflection coming about from the surface of the metal-dielectric interface. A beam of incident light is exceeded by the ATR crystal to be reflected from the interior surface in contiguity with the sensing media. The reflected light comprises of the amount of energy of the incident light except that stretches out within the sensing media. The concentration of biomolecules differs due to chemical reactions, and this results in a topical modification of the encirclement RI close to the sensor surface, which adjusts the SPW propagation constant and, as a result, the SPR angle varies [30], [31]. By interrogating this SPR angle, the sensing medium analyte is detected.

III. MATHEMATICAL MODELLING FOR NUMERICAL SIMULATION

A. MATHEMATICAL MODELING FOR REFLECTIVITY CALCULATION

The prerequisite for investigating the performance of the raised SPR sensor is to measure the resolution of the reflection intensity of the incident light at the output terminal. There is no need for any approximation to apply the transfer matrix method, which is a competent method for measuring the reflectivity of the light bounced back from the metal-dielectric interface of an N-layer model [32]. This technique gives much appropriate result whilst MATLAB programming environment is employed for computing the harmony of SPR modulation. There is a correlation between the tangential component of the propagating SPW with initial limit of $Z = Z_1 = 0$ and the final limit of $Z = Z_{N-1}$. The relationship between aforementioned initial limit and the final limit was presented in [5] by equation 3:

$$\begin{bmatrix} U_1 \\ V_1 \end{bmatrix} = M \begin{bmatrix} U_{N-1} \\ V_{N-1} \end{bmatrix} \quad (3)$$

Whither U_1 and V_1 depict the tangential elements of the electric and magnetic fields, respectively, at the limiting surface. In addition, the analogous bounds owing to the limit of the N^{th} layer are U_{N-1} and V_{N-1} . The characteristics matrix of this composite design is the M_{ij} . In this way, the equation 4 to 7 are used to define the plane-polarized light at different boundaries of the architecture [5]:

$$M_{ij} = \left(\prod_{k=2}^{N-1} M_k\right)_{ij} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \quad (4)$$

With,

$$M_k = \begin{pmatrix} \cos \beta_k & -(i \sin \beta_k)/q_k \\ -iq_k \sin \beta_k & \cos \beta_k \end{pmatrix} \quad (5)$$

where,

$$q_k = \left(\frac{\mu_k}{\varepsilon_k}\right)^{1/2} \cos \theta_k = \frac{(\varepsilon_k - n_1^2 \sin^2 \theta_1)^{1/2}}{\varepsilon_k} \quad (6)$$

$$\beta_k = \frac{2\pi}{\lambda} n_k \cos \theta_k (z_k - z_{k-1}) = \frac{2\pi d_k}{\lambda} (\varepsilon_k - n_1^2 \sin^2 \theta_1)^{1/2} \quad (7)$$

Here, d_k explains the density of the ledges that are thought towards the z-axis. Likewise, this can be resolved by determining a dielectric constant and RI in the kth layer, which could be presented separately using ϵ_k and η_k . The reflection coefficient for plane-polarized incident light is expressed by equation 8 [5]:

$$r_p = \frac{(M_{11} + M_{12}q_N)q_1 - (M_{21} + M_{22}q_N)}{(M_{11} + M_{12}q_N)q_1 + (M_{21} + M_{22}q_N)} \quad (8)$$

At last, the reflection intensity for plane-polarized light is given by equation 9 [5]:

$$R_p = |r_p|^2 \quad (9)$$

B. PERFORMANCE EVALUATING PARAMETERS OF SPR SENSOR

It is important to evaluate the resonance angle or SPR point for the respective analyte or sensing medium RI to investigate the quality of the proposed sensor. The point of SPR or resonance angle is the point where the minimum light reflectance is detected analogous to the angle of the incident. Sensitivity, quality factor (QF), and detection accuracy (DA) are the key performance evaluating parameters of SPR based sensors that ought to be as exalted as contingent for a decent sensor. The concept of sensitivity (S) of the SPR based sensor can be illustrated as the variation in resonance angle (or SPR point) due to bimolecular adsorption in the sensing medium that causes an alternation in the RI. The sensitivity (S) is expressed by equation 10 and the dimension of this parameter is deg/RIU [3]:

$$S = \frac{\Delta\theta_{SPR}}{\Delta n_a} \quad (10)$$

When investigating the characteristics of the SPR sensors, it is crucial to reduce the FWHM of the SPR curves to retain the resonance dip fixation as secure as possible. One of the vital performance parameters relevant to the FWHM is the detection accuracy which can be described as the inverse of the FWHM, and the dimension of this parameter is 1/deg as defined by equation 11 [3]:

$$DA = \frac{1}{FWHM} \quad (11)$$

Another measurement scale for getting clear concept of the sensing efficiency is the figure of merit (FOM), also known as the quality factor (QF) of the sensor. It is determined as the ratio of the sensitivity to the sensor's FWHM, dimensioned in RIU⁻¹, and is described by the equation 12 [33]:

$$FOM = \frac{S}{FWHM} \quad (12)$$

Selectivity, one of the performance measuring indicators, determines whether the sensor can detect a certain analyte. As it is related to the experimental results, it is avoided in this study [33]–[35]. Another important issue related to sensor is cross-sensitivity effect. When any element from the environment interferes with the sensor surface, causing

the sensor to react even if the desired sample is not there, is known as cross-sensitivity. It develops in an SPR sensor when a single substance is employed to survey different features concurrently, such as magnetic fluid for monitoring temperature and magnetic field [37]. Unfortunately, it is very difficult to develop a sensor that will not respond to anything other than the target samples. It may be presumed to develop a hydrogen sulfide (H₂S) sensor to only read H₂S, but there are other gases like H₂ in the vicinity that can generate readings on this sensor. It cannot be totally eradicated, however it can be slowed down using various strategies such as filters. In this research, a numerical investigation is utilized to suggest an SPR sensor for detecting analytes with RI greater than 1.33, and the analysis of cross-sensitivity effect is deliberately excluded because it mostly affects gas sensing performance.

IV. RESULTS AND DISCUSSION

A simple metallic layer is mostly offered by the Kretschmann geometry-based sensors to excite the surface plasmon polaritons (SPPs) of the conventional architecture. By employing BK7 glass prism, the change in SPR angle is found as 0.68 deg for an analyte RI variation of 0.005 from 1.330 to 1.335, resulting in a sensitivity of 136 deg/RIU for the conventional Au flourished sensor as shown in Fig. 2. On the contrary, for enhancing the performances of the SPR based sensors, different hybrid structured SPR sensors utilizing 2D materials are simulated and the performances are evaluated in this paper.

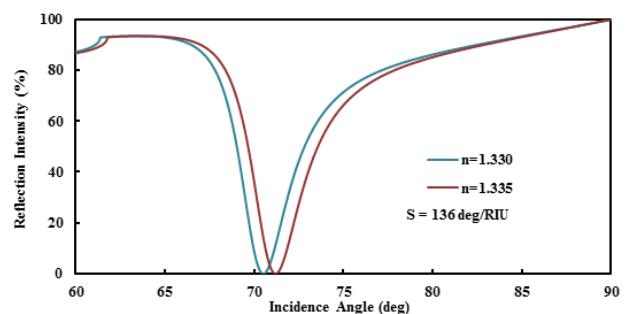


FIGURE 2. Reflectivity variation of conventional SPR sensor [BK7-Au (50 nm)-Analyte] for analyte RI of 1.330 and 1.335.

In this work, a sensor with improved performance is observed with the accession of 2D TMDC PtSe₂, WSe₂, and BP in between the plasmonic metallic layer and the sensing surface in the structure. The resonance condition is obtained when the phase of incident light matches with the phase of propagating SPW in SPR sensors. This criterion can be met theoretically if the incident light's propagation constant in the direction of the SPW is identical to the propagation constant of the SPW where maximum evanescent field absorption is seen, resulting in a strong SPW generation [38]. The propagation constant β_{ev} can be used to characterize the propagating evanescent wave as follows [33], [39]:

$$\beta_{ev} = \frac{2\pi}{\lambda_{light}} n_{prism} \times \sin\theta \quad (13)$$

TABLE 1. Analysis of different architectures of SPR sensor utilizing TMDC 2D materials (e.g. PtSe₂, WSe₂) and BP to obtain a hybrid structure with enhanced performances.

Sl. No.	Structure	Thickness of PtSe ₂ (nm)	No. of WSe ₂ layer(p)	No. of BP layer(q)	R _{min} (%)	Θ _{SPR} (deg) for n=1.33	ΔΘ _{SPR} (deg) for Δn=0.005	S (deg/RIU)	FWHM (deg)	FOM (RIU ⁻¹)
1.	BK7-Au	0	0	0	0.0064	70.54	0.68	136	3.80	35.79
2.	BK7-Au-PtSe ₂	4.4	0	0	46.76	76.01	0.76	152	14.4	10.56
3.	BK7-Au-PtSe ₂	3.6	0	0	31.86	75.00	0.83	166	11.6	14.31
4.	BK7-Au-PtSe ₂	2	0	0	12.63	72.93	0.78	156	7.4	21.08
5.	BK7-Au-WSe ₂ -PtSe ₂	4.4	1	0	52.03	77.70	0.67	134	15.1	8.87
6.	BK7-Au-WSe ₂ -PtSe ₂	3.6	1	0	38.14	77.01	0.84	168	13.3	12.63
7.	BK7-Au-WSe ₂ -PtSe ₂	2	1	0	17.81	74.84	0.86	172	9.4	18.30
8.	BK7-Au-PtSe ₂ -BP	4.4	0	1	49.07	77.04	0.73	146	14.7	9.93
9.	BK7-Au-PtSe ₂ -BP	3.6	0	1	33.80	76.15	0.85	170	12.4	13.70
10.	BK7-Au-PtSe ₂ -BP	2	0	1	13.53	73.93	0.86	172	8.1	21.23
11.	BK7-Au-PtSe ₂ -WSe ₂ -BP	2	1	1	19.75	76.15	0.90	180	10.2	17.65
12.	BK7-Au-WSe ₂ -PtSe ₂ -BP	2	1	1	19.50	76.05	0.92	184	10.2	18.04

where λ_{light} , n_{prism} , θ indicate the incident light wavelength, RI of the prism coupler, and incidence angle of light at the metal surface, separately. The following equation characterizes the SPW for a conventional SPR sensor with a single layer of plasmonic material and dielectric medium (or sensing medium) [33]:

$$\beta_{SPW} = \beta_f \sqrt{\frac{\epsilon_m \epsilon_a}{\epsilon_m + \epsilon_a}} \tag{14}$$

where λ_{light} , ϵ_m and ϵ_a indicate the wave vector of light at free space, dielectric constants of plasmonic material and sensing medium, respectively. Equation 14 can also be modified in terms of RI as follows [33]:

$$\beta_{SPW} = \frac{2\pi}{\lambda} \sqrt{\frac{n_m^2 n_a^2}{n_m^2 + n_a^2}} \tag{15}$$

where the RI of plasmonic materials (n_m) and sensing medium (n_a) are connected to the dielectric constants as $n_m^2 = \epsilon_m$ and $n_a^2 = \epsilon_a$, respectively. Equation 13 and 15, connected by equation 16, can be used to find the SPR angle under resonance conditions:

$$\theta_{SPR} = \text{Sin}^{-1} \left(\frac{1}{n_{prism}} \sqrt{\frac{n_m^2 n_a^2}{n_m^2 + n_a^2}} \right) \tag{16}$$

The greater the change in SPR angle due to the same fluctuation in RI of the sensing medium, the higher the sensitivity is, as shown in equation 10. In addition, equation 16 shows that the SPR point is dependent on the plasmonic materials' RI for a given prism coupler and analyte RI. The heterostructure of PtSe₂ with Wse₂ and BP in the raised sensor alters the SPR angle according to equation 17 [40]:

$$\theta_{SPR} = \text{Sin}^{-1} \left(\frac{1}{n_{prism}} \sqrt{\frac{n_{Au}^2 n_{WSe_2}^2 n_{PtSe_2}^2 n_{BP}^2 n_a^2}{n_{Au}^2 + n_{WSe_2}^2 + n_{PtSe_2}^2 + n_{BP}^2 + n_a^2}} \right) \tag{17}$$

As a result of this change in effective RI, the shift in SPR angle increases for the same variation in RI of the sensing medium, resulting in an improvement in sensor's sensitivity. To get the optimized sensors, different architecture, as well as the structural parameters, were altered and analyzed which have been listed in Table 1.

It can be visualized after observing Table 1 that the addition of PtSe₂ layer with the conventional architecture of SPR sensors improves performances but the sensitivity of them is quite low. Therefore, the structures were further modified with the accession of BP and WSe₂. It can be observed that the addition of the only WSe₂ in between the Au and PtSe₂ layer can slightly improve the sensitivity of the structures. For the addition of a single layer of WSe₂, the sensitivity is found as 134 deg/RIU, 168 deg/RIU, and 172 deg/RIU, respectively, for 4.4 nm, 3.6 nm, and 2 nm thickness of PtSe₂. On the other hand, another structure employing a single layer of BP over the PtSe₂ reveals the sensitivity of 146 deg/RIU, 170 deg/RIU, and 172 deg/RIU, respectively, for 4.4nm, 3.6 nm, and 2 nm thickness of PtSe₂. The structure was further modified with the insertion of different layers of WSe₂, PtSe₂, and BP in the structure and the performance was observed. It can be witnessed that the structures e.g., BK7-Au-PtSe₂-WSe₂-BP and BK7-Au-WSe₂-PtSe₂-BP with a single layer of WSe₂ and BP improves the sensitivity up to 180 deg/RIU and 184 deg/RIU, respectively, for 2 nm thickness of PtSe₂. After that, the structural parameters e.g., number of WSe₂ and BP layers were altered for optimizing the structure to get better performances of the sensor. The reflectivity variation for the architecture of BK7-Au-WSe₂-PtSe₂-BP and the characteristics of SPR curves was observed due to change in the number of layers of WSe₂ and BP as shown in Fig. 3 where the solid and dotted line reflecting the analyte RI of 1.330 and 1.335, respectively. From Fig. 3, it can be noticed that, with 50 nm thickness of Au and 2 nm thickness of PtSe₂, the SPR condition changes due to a change in the analyte RI as well as for different

TABLE 2. Performance analysis of the proposed hybrid structured SPR sensor for different layers of WSe₂ (*p*) and BP (*q*) to optimize the structural parameters.

Sl. No.	Structure	Thickness of PtSe ₂ (nm)	No. of WSe ₂ layer (<i>p</i>)	No. of BP layer (<i>q</i>)	R _{min} (%)	Θ _{SPR} (deg) for 1.33	ΔΘ _{SPR} (deg) for Δn=0.005	S (deg/RIU)	FWHM (deg)	FOM (RIU ⁻¹)
1.	BK7-Au-WSe ₂ -PtSe ₂ -BP	2	1	1	19.50	76.05	0.92	184	10.2	18.04
2.	BK7-Au-WSe ₂ -PtSe ₂ -BP	2	1	2	21.92	77.40	0.98	196	11.0	17.82
3.	BK7-Au-WSe ₂ -PtSe ₂ -BP	2	1	3	25.54	78.89	1.00	200	11.3	17.70
4.	BK7-Au-WSe ₂ -PtSe ₂ -BP	2	1	4	31.11	80.43	0.93	186	12.1	15.37
5.	BK7-Au-WSe ₂ -PtSe ₂ -BP	2	2	3	40.66	81.32	0.68	136	12.7	10.71

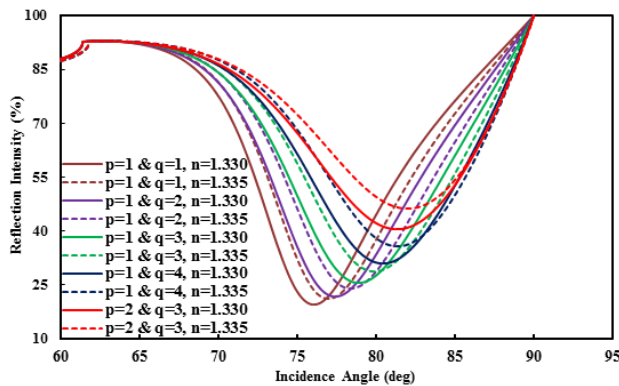


FIGURE 3. Variation of reflectivity (*R_{min}*) and SPR angle (*Θ_{SPR}*) of the proposed structure (BK7-Au-WSe₂-PtSe₂-BP) for different layers of WSe₂ (*p*) and BP (*q*) due to variation of RI of 1.330 and 1.335.

layers of WSe₂ and BP indicated by *p* and *q*, respectively. For *p* = 1 & *q* = 1, *p* = 1 & *q* = 2, *p* = 1 & *q* = 3, *p* = 1 & *q* = 4 and *p* = 2 & *q* = 3, the SPR conditions were found at a light incident angle of 76.05°, 77.40°, 78.89°, 80.43° and 81.32°, respectively for an analyte RI of 1.33. Due to the change in analyte RI from 1.33 to 1.335, the shift in SPR angle was observed as 0.92°, 0.98°, 1.00°, 0.93° and 0.68° for the same incidence angle configurations. Considering this change in the SPR angles, the sensitivity of different configurations was calculated in Table 2 by using equation 10.

From Table 2, it can be noticed that with a single layer of WSe₂ the sensitivity of the sensor was calculated as 184 deg/RIU, 196 deg/RIU, 200 deg/RIU, and 186 deg/RIU, for 1, 2, 3, and 4 layers of BP, respectively. It can be concluded that for 3 layers of BP, the sensor shows better sensitivity. Considering 3 layers of BP, the WSe₂ layer was changed. It can be noticed from Table 2 that increasing the layers of WSe₂ degrade the sensitivity of the sensors. Finally, the sensor was optimized with 50 nm thickness of Au, a single layer of WSe₂, 2 nm thickness of PtSe₂, and three layers of BP. The reflectivity variation of the optimized structure for analyte RI of 1.33 and 1.335 is shown in Fig. 4 and other

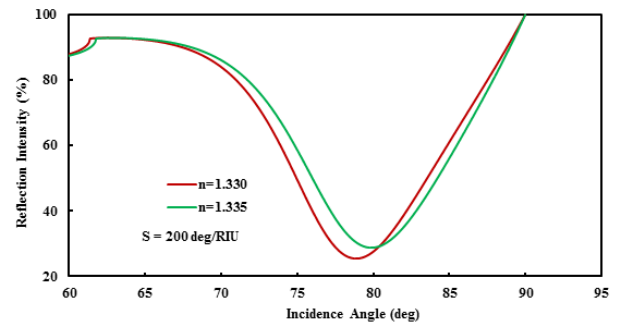


FIGURE 4. Variation of reflectivity (*R_{min}*) and SPR angle (*Θ_{SPR}*) of the proposed sensor for analyte RI of 1.330 and 1.335.

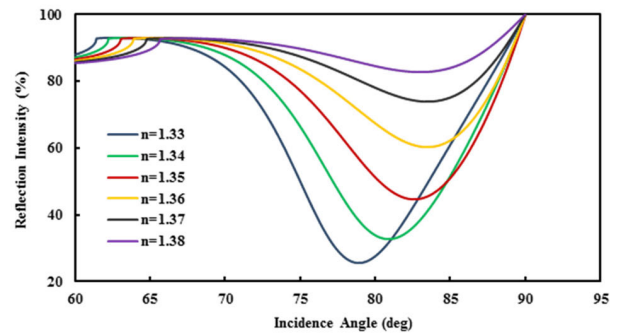


FIGURE 5. Variation of reflectivity (*R_{min}*) and SPR angle (*Θ_{SPR}*) of the proposed sensor due to change in sensing medium RI ranging from 1.33 to 1.38.

performance parameters e.g., FWHM, DA, and FOM for the optimized structure are calculated as 11.3 deg, 0.09 deg⁻¹ and 17.70 RIU⁻¹, respectively.

The performances of the proposed sensor was investigated for both gas and liquid sensing. The SPR point was computed at angles of 45.15°, 45.81°, 46.47°, 47.15°, 47.84°, 48.55°, and 49.26 for analyte RI of 1.00, 1.01, 1.02, 1.03, 1.04, 1.05, and 1.06, respectively, while testing the sensor's sensitivity for analyte RI of 1.00 to 1.05. For analyte RI of 1.00, 1.01, 1.02, 1.03, 1.04, and 1.05, the sensor's sensitivity

TABLE 3. Comparison of the proposed hybrid structured SPR sensor with some prior reported sensors.

Ref. and reported year	Configuration of the sensors	Sensitivity (deg/RIU)	FOM (RIU ⁻¹)
[15] 2020	BK7/Ag/PtSe ₂	162	14.93
[15] 2020	BK7/Au/PtSe ₂	165	14.12
[16] 2020	BK7/Au/WSe ₂ /Graphene	178.87	27.86
[17] 2020	SF11/Au/MoS ₂ /WS ₂ /WSe ₂	142	-
[20] 2018	SF6/ Chromium/Au/BP/WS ₂	187	-
[41] 2020	SF11/Au/MoS ₂ /graphene	130	17.02
[42] 2021	SF10/Au/ α -SnSe ₂ /Phosphorene	96.43	12.36
Proposed Sensor	BK7/ Au/ WSe ₂ /PtSe ₂ /BP	200	17.70

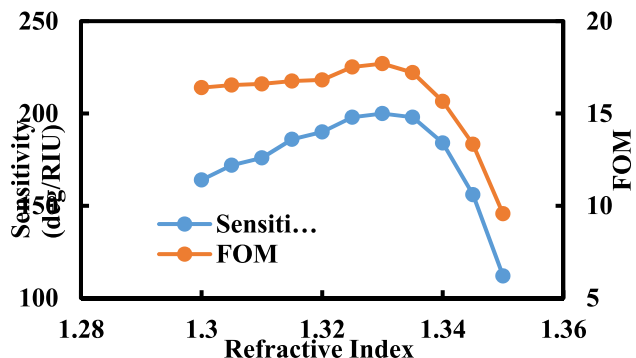


FIGURE 6. Sensitivity and FOM of the proposed SPR sensor as function of sensing medium RI ranging from 1.30 to 1.35.

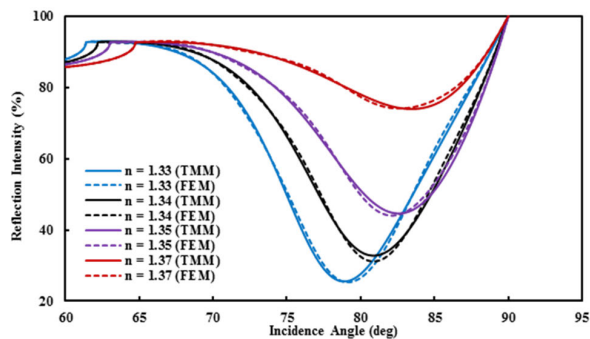


FIGURE 7. Reflectivity curves of the proposed sensor found from TMM (indicated by solid line) and FEM (indicated by dotted line) based analysis for sensing medium RI of 1.33, 1.34, 1.35, and 1.37.

was computed as 66 deg/RIU, 66 deg/RIU, 68 deg/RIU, 69 deg/RIU, 71 deg/RIU, and 71 deg/RIU respectively. Further investigation of the sensor as a potential gas sensor is thus avoided due to its low sensitivity. Then the operating region of the proposed sensor as a liquid analyte sensor was determined by altering the RI (n) of the sensing medium and Fig. 5 show the variation of reflectivity for different RIs of the sensing medium. It can be observed that the proposed sensor will be able to detect the analyte ranging from 1.33 to 1.38 where the SPR angles were found as 78.89°, 80.88°, 82.58°, 83.45°, 83.46° and 82.98° for n = 1.33, n = 1.34, n = 1.35, n = 1.36, n = 1.37 and n = 1.38, respectively. As the RI of the analyte increases, the SPR angle also increases. The SPR angle tends to be saturated after a certain point, as displayed in Fig. 5 for an analyte RI of 1.38, which is the sensor's

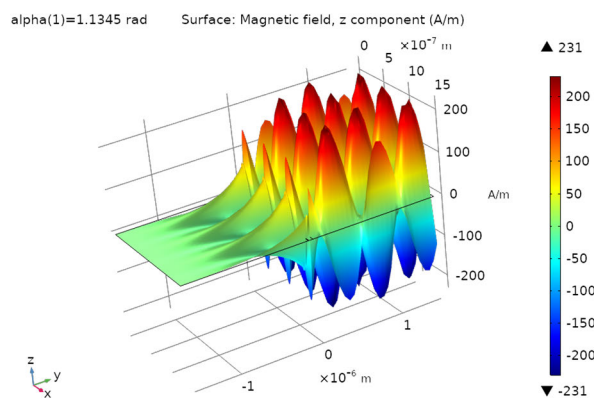


FIGURE 8. Light penetration through the optimized structure of the proposed sensor for an analyte RI of 1.33.

maximum operating point. Also, Fig. 6 shows the sensitivity as well as the FOM of the proposed sensor as a function of the sensing medium RI ranging from 1.30 to 1.35. Observing the figure, it can be visualized that the proposed sensor shows the maximum possible sensitivity of 200 deg/RIU with a FOM of 17.70 RIU⁻¹. The use of a hybrid structure of two-dimensional materials affects the sensor's absorption capability. It also changes the effective RI of the sensors, which is linked to the sensor's sensitivity. When a hybrid structure of two-dimensional materials (WSe₂-PtSe₂-BP) is combined with SPR active gold, the effective RI of the sensor changes resulting in a higher shift in SPR angle for the same variation in sensing medium RI. As a result an enhancement in sensor's sensitivity is observed with an adoptable detection accuracy.

In order to observe the penetration of evanescent wave through sensor, the optimized structure of the proposed sensor found from the TMM was further simulated and analyzed using the finite element method (FEM) based COMSOL multiphysics software. The reflectivity variations for different analyte RIs of the sensing medium were calculated and plotted in Fig. 7 where the dotted line indicates the reflectivity curves found from the finite element analysis (FEA) and the solid lines are obtained from TMM based analysis. It can be noticed that the FEA and TMM based analyses produce nearly identical results, indicating that the simulated structure is valid for TMM analysis. The evanescent wave as well

as light penetration through the optimized structure of the proposed sensor for an analyte RI of 1.33 is displayed in Fig. 8.

Finally, in Table 3, the performance of the proposed hybrid structured SPR sensor is compared in terms of sensitivity and FOM to that of other recently reported sensors. It is impressive that the proposed sensor outperforms the previously reported sensors with an outstanding FOM, particularly in terms of sensitivity. Implementation of hybrid heterostructure of 2D materials in the proposed sensor alters the SPR condition that results in improved performance.

V. CONCLUSION

A hybrid model of Kretschmann configuration based sensor formation utilizing 2D materials e.g., PtSe₂, WSe₂, BP has been theoretically explored in this paper by using the transfer matrix method. Different configurations of SPR based sensors are designed and analyzed to propose a sensor with improved performance. In addition, the performances of the proposed sensor have been investigated by altering the structural parameters e.g., the thickness of PtSe₂, WSe₂, BP applied over the plasmonic metal substrate. For enhancing the sensor's sensitivity with an adoptable FOM, an unprecedented sensor has been designed and proposed where an enhanced sensitivity is obtained with the addition of different 2D materials that alters the effective refractive index (RI) of the sensor ensuring more interaction of evanescent fields to the surface plasmons, in between the sensing medium and plasmonic material. The structure of the proposed sensor consists of a low refractive index BK7 prism that acts as a light coupler with a 50 nm thickness of gold layer over it. Then an optimized hybrid structure is formed with a single layer of WSe₂, 2nm of PtSe₂ and, 3 layers of BP which is applied in between the sensing medium and the gold layer. With this optimized structure, the sensor shows a maximum sensitivity of 200 deg/RIU with a FOM of 17.70 RIU⁻¹. As the sensor delivers promising sensitivity with a skimpy diminished FOM, it is persuaded that the sensor may be used in several petitions of biological and biochemical sensing applications.

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