



Sensitivity enhancement of biosensor (SPR) with PtSe_2 using Au–Si–Au thin films

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Received: 25 January 2024 / Accepted: 16 March 2024 / Published online: 11 April 2024
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Abstract In this study, we presented a novel structure for a highly sensitive surface plasmon resonance (SPR) sensor, we propose a structure which contains six layers: BK7 prism glass, Gold thin film, Silicon sheets, Gold thin film, using transition figure of merit (FOM) 16.43 RUI^{-1} metal dichalcogenides 2D PtSe_2 layer and sample medium. We have been optimizing the thickness of each layer. The highly performance parameters in this biosensor structure are provided in terms of sensitivity (S), detection accuracy (DA), quality factor (QF) and figure of merit (FOM). Here, the addition of the hybrid *Silicon*— PtSe_2 layer between two gold films increased the sensitivity, but we observed the (DA)

and (QF) is decreased. We find the full at half maximum also decreased. We investigated the effect of gold thickness. The maximum sensitivity $200^\circ/\text{RIU}$ and is gained with 35 nm Gold film, 5 nm thickness Silicon and 2 nm PtSe_2 layer, we can be obtained also the configuration with 60 nm Gold thin film and 3 nm thickness Silicon (6 layer) delivers a maximum sensitivity (S) of $206^\circ/\text{RIU}$ with figure of merit (FOM) of 24.03 RUI^{-1} . Our novel structure is optimized for a highly sensitive surface plasmon resonance (SPR) sensor.

Keywords Surface plasmon resonance · Thickness optimization · Biosensor · Silicon · PtSe_2 · Sensitivity

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Introduction

Surface plasmon resonance phenomena occur optically, which achieves more excellent detection sensitivity [1]. Surface plasmons (SP) are free quantities of surface oscillations, obtained at the surface of a thin metallic film, the collective charge density oscillations propagate confined to the metallic dielectric interface. When the wave vector of an incident light couples with the wave vector of the evanescent wave, it is called a surface plasmon resonance (SPR) [2, 3]. The prism coupler used by Kretsch Amann's ATR. In this configuration, the base of the prism is directly connected to the metal [4], but in Otto's configuration it used a very thin air gap between the prism and the film metal [5], for the purpose of exciting the surface plasmon. SPR sensors have received increasing attention due to their recent applications such as nanofibers and photonic crystal fiber [6, 7], solar cells [8], to detect specific bio-sensing [9, 10], used for detecting fat and melamine concentration milk [11]. Detection of chikungunya, virus dengue virus and diagnosis of novel coronavirus SARS-CoV-2 [12–14], designed for cancer cell detection

[15, 16] biochemical interaction and detecting nano-objects in solution [17, 18] including medical diagnosis [19, 20], to detect disease in human teeth [21].

However, the SPR-based sensor is an excellent technique for sensing due to its important advantages such as high sensitivity, faster response, the dynamics of a reaction to follow in real time and the wide range of refractive index of the analyte [22–24]. Although SPR sensors use a variety of materials, recent research is interested in traditional transition metal dichalcogenides (TDM), because of their perfect electronic and optical properties. Recently, traditional (TDMs) have been intensively investigated theoretically and experimentally to demonstrate that some noble metals can form a layered structure with S and Se, of which $PtSe_2$ is one of the most important properties, such as the largest band gap of (1.2 eV) for a monolayer of semiconductors, going from a bulk semi-metallic $PtSe_2$ with zero band gap its strong inter-layer interaction. On the other hand, the $PtSe_2$ can also offers inertness to chemical agents and resilience to toxicity, making it a suitable material for sensing applications [25].

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

However, Silicon is getting more and more attention last 10 years due to its low cost. The addition of silicon in the structure SPR layer is capable of raising its sensitivity [26], Verma et al. used the silicon between the Gold and graphene layer in the SPR sensor was the highest sensitivity [27]. Ougang et al. have proposed the structure base for Silicon and TMDs on Gold film, and it was achieved with a more excellent sensitivity [28]. Rajeev et al. proposed SPRsensor-based Silicon and two-dimensional MXene (Ti_3C_2TX) to increase the sensitivity [29]. The employing of the Si nanomaterials has been theoretically improved the sensitivity [15]. $PtSe_2$ over Ag and Au has demonstrated significant for improving sensitivity of sensor up to 162 deg/RIU and 265 deg/RIU, respectively. Rahman et al. are designed a novel structure (Ag– $PtSe_2$ – WSe_2) there sensitivity are 194 deg/RIU and 187 deg/RIU, respectively [30]. M. Mahabubur et al. have been proposed (Au– WSe_2 – $PtSe_2$ –BP) for improving the sensitivity up to 200 deg/RIU [31]. In this context of the present paper, we propose the traditional SPR biosensor schema based six layers on Silicon– $PtSe_2$ coated biosensor. It was introduced in order to analyze and characterize some keys such as change of resonance angle θ_{res} , minimum reflectance (R_{min}), FWHM, detection accuracy (DA), sensitivity (S) and FOM. We suggest a novel structure used numerical simulations of transfer matrix method (TMM); Here the architect-based Au/Si/Au/ $PtSe_2$ explored to improve its sensitivity.

It found a great advancement of the sensitivity of SPR by using the modified schema. These papers are presented as follows, the mathematical expression is in Sect. 2, the results and discussion are discussed in Sect. 3. Finally, the conclusion and necessary references are arranged at the end.

Mathematical background

This proposed structure is a modified Kretschmann model, as shown in Fig. 1. We used an SPRsensor using a multilayer composition consisting of a metal (Gold) film deposited at the base of the BK7 glass prism, silicon (Si) is attached with Gold. film, and the exterior of the silicon layer is also kept in direct contact with another metal layer. The biomolecular recognition element consists of the $PtSe_2$ layer, which has a monolayer thickness of 0.375 nm [31].

The refractive index of the biological sample is considered to vary from 1.33 [32]. The BK7 glass prisms is characterized by the following dispersion relation (1) [33]:

where λ the wavelength (μm).

The complex RI of Gold at different wavelengths can be calculated from the Drude-Lorentz model [34]:

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

Here $\lambda_c = 2.4511 \times 10^{-5} m$ and $\lambda_p = 1.6826 \times 10^{-7} m$ are the collusion and the plasma wavelength of Gold,

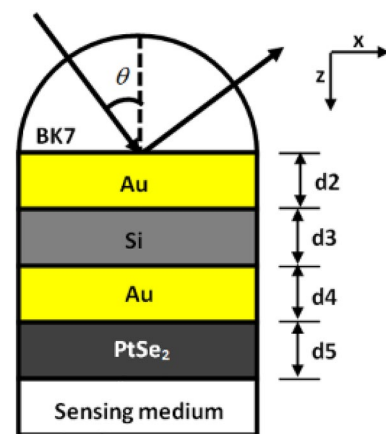


Fig. 1 Multilayer stack diagram of the biosensor based on Si and $PtSe_2$

respectively. The Silicon layer refractive index can be calculated using the following equation [35].

$$n_{Si} = A + A_1 e^{-\lambda t_1} + A_2 e^{-\lambda t_2} \quad (3)$$

where: $A = 3.44904$, $A_1 = 2271.88813$, $A_2 = 3.39538$, $t_1 = 0.058304$ and $t_2 = 0.30384$ at λ wavelength in μm . The complex dielectric value of PtSe_2 depends on the thickness at wavelength of 633 nm, it is calculated using from the literature [36, 37].

We employ the matrix method to calculate the reflectance of the reflected light of the six-layer model. This matrix method is efficient and does not require any approximation. In this structure, all the layers are structured in the Z direction, each layer is characterized by the thickness (dk) and the constant optics of the metal and the dielectric. The relation between the tangential components of the electric field (E) and the tangential components of the magnetic fields (H) at the first and the final layer is given by [38].

$$M = \prod_{G=2}^{G-1} M_G = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \quad (4)$$

$$M_G = \begin{bmatrix} \cos \delta_G & \frac{-\sin \delta_G}{q_G} \\ -iq_G \sin \delta_G & \cos \delta_G \end{bmatrix} \quad (5)$$

where η_G is the phase factor of the thin film and δ_G is the phase thickness and is determined as:

$$q_G = \frac{\sqrt{n_G^2 - k_G^2 - n_p^2 \sin^2 \theta_i - 2in_G k_G}}{\epsilon_G} \quad (6)$$

$$\delta_G = \frac{2\pi}{\lambda} d_G \sqrt{n_G^2 - k_G^2 - n_p^2 \sin^2 \theta_i - 2in_G k_G} \quad (7)$$

θ_i is the angle of incidence, and n_G, k_G are constant optic of the complex refractive index and d_G the thickness of the metal layer.

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

The reflectance (R) is given by:

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

Results and discussion

The optimization of sensitivity, detection accuracy and quality factor were considered as the main performance parameters of the excellent *SPR* sensor. The sensitivity (S) can be defined as the ratio of the change in the resonance angle (θ_{SPR}) to the change in the refractive index of the sensing region:

$$S = \frac{d\theta_{SPR}}{dn_{biosample}} \quad (10)$$

The detection accuracy (DA) is a known as the ratio of the shift resonance angle (θ_{SPR}) to the full width at half maximum of the resonance plasmon curve as can be seen in the following relation:

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

Another important parameter of interest is the figure of merit (FOM) that is determine as the ratio of the reflectance curve of sensitivity to the $FWHM$ [39]:

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

Three schematic structure and their performance parameters of the *SPR* sensor reflectance curve for each structure as a function of the incident angle of sensing medium summarized in Table 1.

Figure 2a; show the movement of resonance angle is 1° with small increment in $RI = 0.005$ for $d(\text{Au}) = 35$ nm, $d(\text{Si}) = 5$ nm. It can see the calculated sensitivity from Eq. (10) of conventional sensor is $200^\circ/\text{RIU}$; after increasing thickness of Gold and decreasing thickness of silicon $d(\text{Au}) = 60$ nm, $d(\text{Si}) = 3$ nm in conventional *SPR* sensor. It can observe that the sensitivity achieved $206^\circ/\text{RIU}$ shown in Fig. 2b.

Table 2; presents the values of minimum reflectance (R_{min}), sensitivity (S), full width half maximum ($FWHM$), detection accuracy (DA), and figure of merit (FOM) at the

Table 1 Performance parameters of *SPR* sensor reflectance curve for different structure

| Sensor structure used | R_{min} | Sensitivity ($^\circ\text{RIU}^{-1}$) | $FWHM$ ($^\circ$) | DA ($^\circ^{-1}$) | FOM (RIU^{-1}) |
|--|-----------|---|---------------------|------------------------|-----------------------------|
| BK7/Au/sensing medium | 0.2693 | 142 | 2.48 | 0.4032 | 57.25 |
| BK7/Au/PtSe ₂ /sensing medium (15) | 0.3515 | 165 | 11.68 | 0.1412 | 14.12 |
| BK7/Au/Si/Au/PtSe ₂ /sensing medium | 0.0254 | 200 | 12.17 | 0.082 | 16.43 |

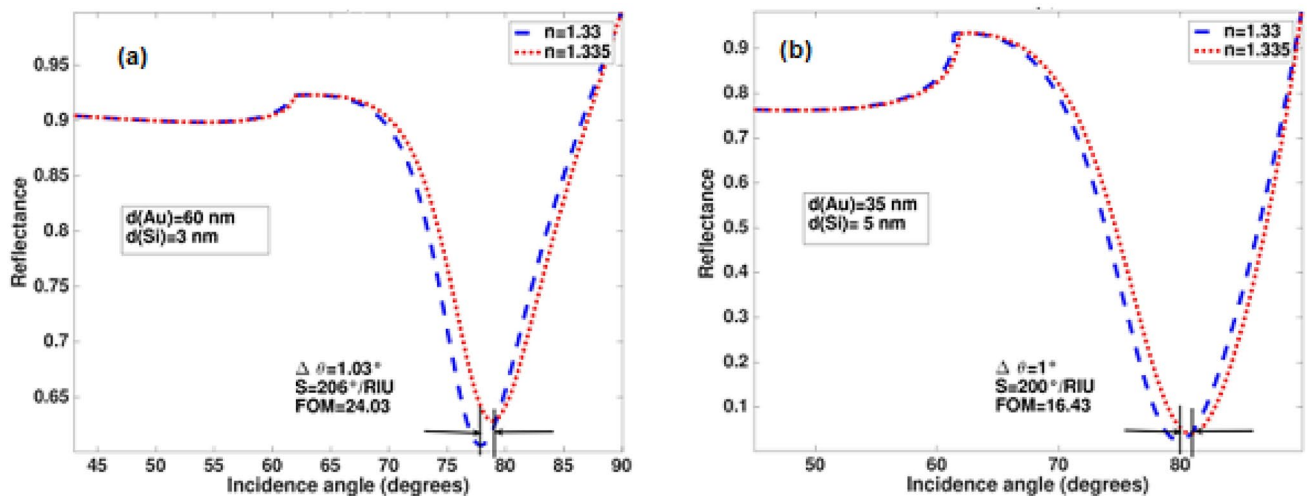


Fig. 2 Reflectance curve as a function of the incident angle for $d(\text{Au})=35$ nm, $d(\text{Si})=5$ nm (a) and $d(\text{Au})=60$ nm, $d(\text{Si})=3$ nm (b)

Table 2 Performance parameter for optimized combination of Gold and Si thickness of proposed SPR

| $d(\text{Au})$ | $d(\text{Si})$ | $d(\text{PtSe}_2)$ | R_{\min} | S | FWHM | DA | FOM |
|----------------|----------------|--------------------|------------|-----|-------|-------|-------|
| 35 | 5 | 0 | 0.099 | 178 | 5.48 | 0.182 | 32.48 |
| 60 | 5 | 0 | 0.375 | 234 | 8.37 | 0.119 | 27.95 |
| 35 | 0 | 2 | 0.005 | 144 | 8.31 | 0.120 | 17.32 |
| 60 | 0 | 2 | 0.531 | 166 | 5.77 | 0.173 | 28.76 |
| 35 | 3 | 2 | 0.026 | 176 | 10.80 | 0.092 | 16.29 |
| 60 | 3 | 2 | 0.606 | 206 | 8.57 | 0.116 | 24.03 |
| 35 | 5 | 2 | 0.025 | 200 | 12.17 | 0.082 | 16.43 |
| 60 | 5 | 2 | 0.725 | 116 | 9.95 | 0.100 | 11.65 |

wavelength 633 nm. the optimization thickness of Gold (Au), Silicon (Si) and the thickness of (PtSe_2) at the illustrated in Fig. 3a–f. It can be observed from Table 2 that the high sensitivity and FOM of the two conventional structure Au/Si/Au/PtSe_2 for combination (1) with thickness Au(35 nm)/Si(5 nm)/Au(5 nm)/ PtSe_2 (2 nm), combination (2) and combination (3) Au(60 nm)/Si(5 nm)/Au(5 nm)/ PtSe_2 (2 nm), for the best combination of SPR biosensor proposed is the structure having Au(60 nm)/Si(5 nm)/Au(5 nm)/ PtSe_2 (2 nm) its property optimum highest sensitivity, optimum figure of merit $206^\circ/\text{RIU}$ and 24.03 respectively. However, the sensitivity, R_{\min} and DA values for combination (1) are $200^\circ/\text{RIU}$, 0.025 and 0.082, respectively. It can be seen in Table 2; that when adding Si layer in the configuration Kretschmann without PtSe_2 layer the sensitivity achieved $234^\circ/\text{RIU}$, this means adding Si layer on sandwich Gold is sufficient to increase the sensitivity enhancement, but biochemical detection needs to use Si and PtSe_2 which greatly allow one to detect analyte.

In this work, the main aim was to optimize the thickness of (PtSe_2), we plotted the change in resonance angle and

the minimum reflectivity with various thickness of Silicon sheets (3, 5 and 7 nm) and the thickness of gold film (30, 35, 40, 45, 50 and 60 nm). Figure 3a–c and d–f show the simulation results of the ($\Delta\theta_{\text{res}}$) and (R_{\min}) respectively.

From Fig. 3a–c we have compared its ($\Delta\theta_{\text{res}}$), it found at the thickness of (PtSe_2) equal to 2 nm the ($\Delta\theta_{\text{res}}$) is as great as for 35 nm thickness of Gold and 5 nm thickness of Silicon ($\Delta\theta_{\text{res}}=1^\circ$) and it can be seen from the plot is the highest that 60 nm thickness of Gold and 3 nm thickness of Silicon ($\Delta\theta_{\text{res}}=1.03^\circ$).

Similarly, Fig. 3d–f shows the minimum reflectivity curves for different thickness of (Gold) with optimized thickness of layer (PtSe_2), and for Fig. 3e at 35 nm thickness of Gold and with 632 nm wavelength, it can be observed from these plots that minimum reflectivity is lower for this case and for Fig. 3d at 60 nm thickness of Gold, it is clear that the minimum reflectivity is still very highest ($R_{\min}=0.60$) which indicates that the SPR in this structure is not strong and the sensing medium is not very remarkable. For a perfect biosensor, ($\Delta\theta_{\text{res}}$) should be high, but at the moment (R_{\min}) should be minimum.

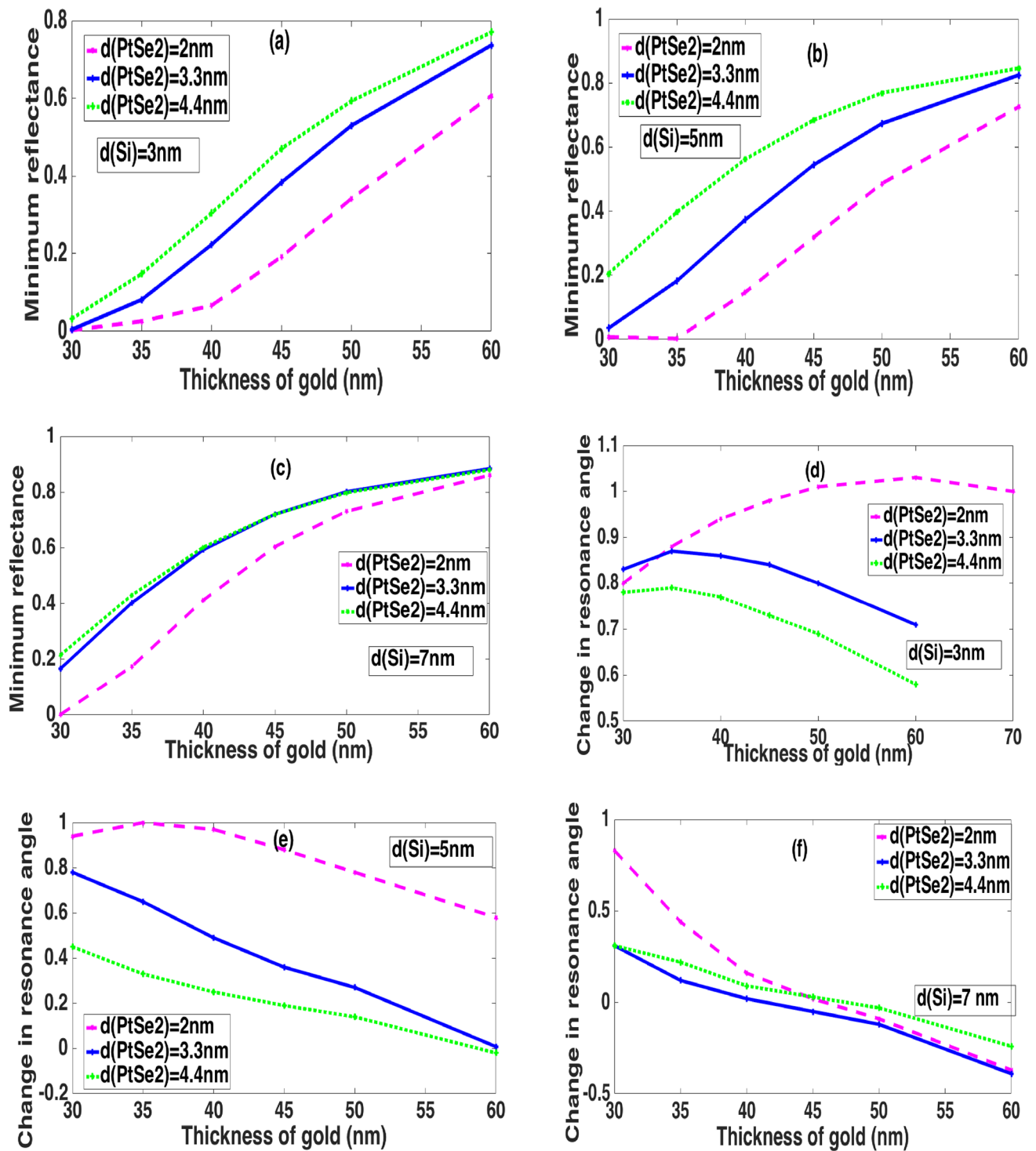


Fig. 3 Minimum reflectivity (R_{min}) resonance angle ($\Delta\theta_{res}$) as a function variation of the thickness of Gold for 2, 3.3, and 4.4 nm of PtSe2 at Si 3, 5, 7 nm

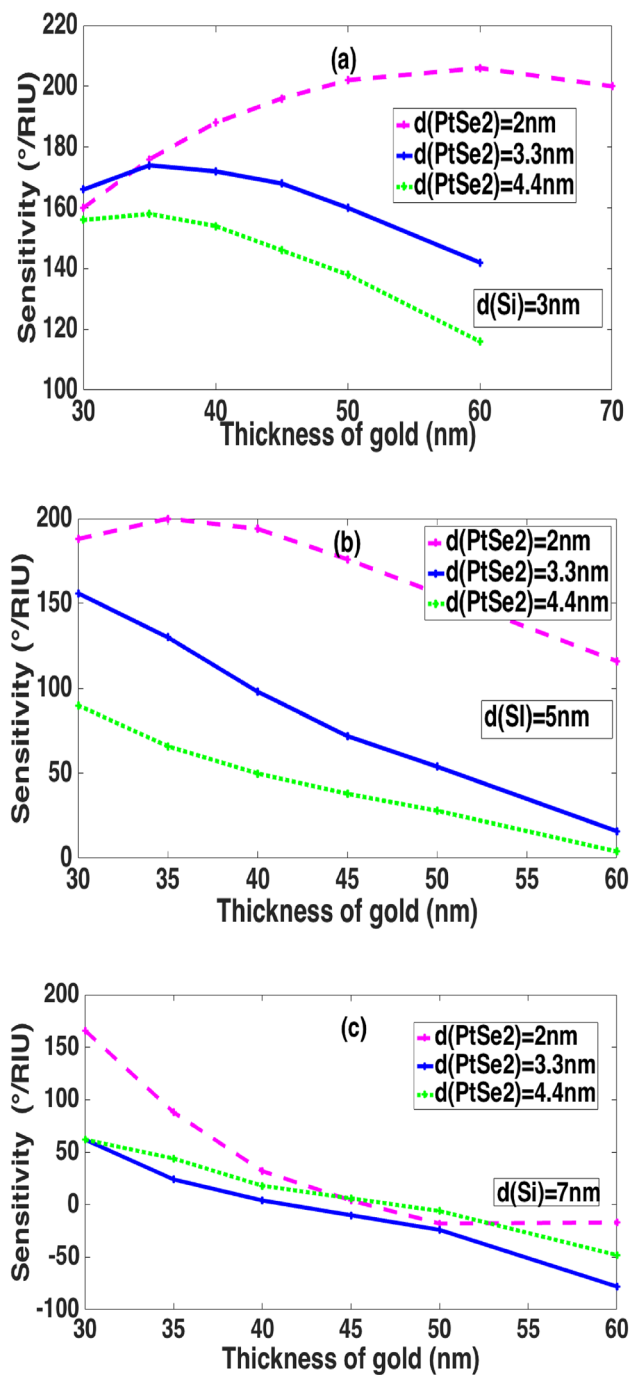


Fig. 4 The sensitivity as a function thickness of Gold and different thicknesses of $PtSe_2$ with **a** $d(Si)=2$ nm, **b** $d(Si)=5$ nm and **c** $d(Si)=7$ nm a wave length 632.8 nm

From Fig. 4, the result shows that change of sensitivity. First, the sensitivity is quasi linear decreasing with the lowest thickness ($PtSe_2$).

The Fig. 4a shows, the sensitivity varies at 60 nm thickness of Gold to $S=206^\circ/RIU$ with thickness of $d(PtSe_2)=2$ nm at $S=142^\circ/RIU$ with thickness of $d(PtSe_2)=4.4$ nm. We may therefore conclude that the sensitivity is best at the lowest ($PtSe_2$) thickness. Secondly, the result illustrates that the sensitivity increased with increasing of gold thickness at 3 nm thickness of Silicon and at the thickness of $d(PtSe_2)=2$ nm.

We can achieve for Fig. 4b at $d(PtSe_2)=2$ nm the sensitivity increase at the maximum $d(Au)=35$ nm equal to $200^\circ/RIU$ and then decreases.

Another important parameter for study a *SPR* biosensor is detection accuracy (*DA*), it is highest for lower thickness ($PtSe_2$), we can see for Fig. 5a the (*DA*) increase with increase of thickness of Gold at $d(PtSe_2)=2$ nm. From Fig. 5b show the (*DA*) increase for maximum and started to decrease.

We calculated the *FOM* by the formula $FOM = S / FWHM$. From this, we can get the *FOM* increase with the increase of thickness of Gold showing a Fig. 6a. For Fig. 6b the *FOM* decrease with the increase of thickness of ($PtSe_2$).

Table 3; shows the comparison among the enhancement of the proposed *SPR* sensor with another existing *SPR* sensor in the literature, and has information on the sensitivity, minimum reflectance, and quality factor at the 633 nm wavelength.

Conclusion

In this study, we have theoretically investigated a novel *SPR* biosensor using (with insertion of) a Silicon layer and $PtSe_2$ layer of the conventional structure to obtain better performances. In this proposed *SPR* biosensor working on the visible light region by using the transfer matrix method. The structure is based on six layers, in which first is a low refractive index BK7 as the coupling prism and insertion the silicon layer and $PtSe_2$ layer between two gold films. The changes of different architect parameters are improving the sensitivity. It found that the change of resonance angle decreases on increasing the thickness of $PtSe_2$, and the present analysis also represents that the *FWHM* decreases up to the extent due to which the quality factor and detection accuracy improve enormously. The result demonstrated that the maximum sensitivity as high as $200^\circ/RIU$ with figure of merit (*FOM*) 16.43 RIU^{-1} can be achieved with structure is designed for gold (35 nm), Silicon (5 nm) and $PtSe_2$ (2 nm), where the highest sensitivity $206^\circ/RIU$ can be obtained for Gold (60 nm), Silicon (3 nm) and $PtSe_2$ (2 nm). Additionally, the maximum figure of merit (*FOM*) is 16.43 RIU^{-1} .

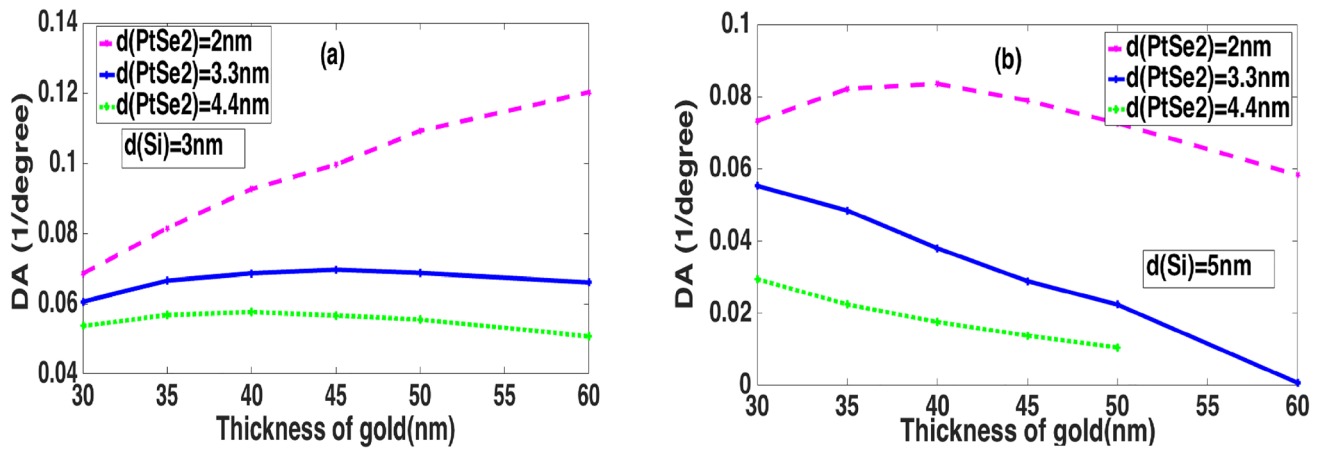


Fig. 5 The DA as a function thickness of Gold $d(\text{Si}) = 3 \text{ nm}$ (a) and $d(\text{Si}) = 5 \text{ nm}$ (b)

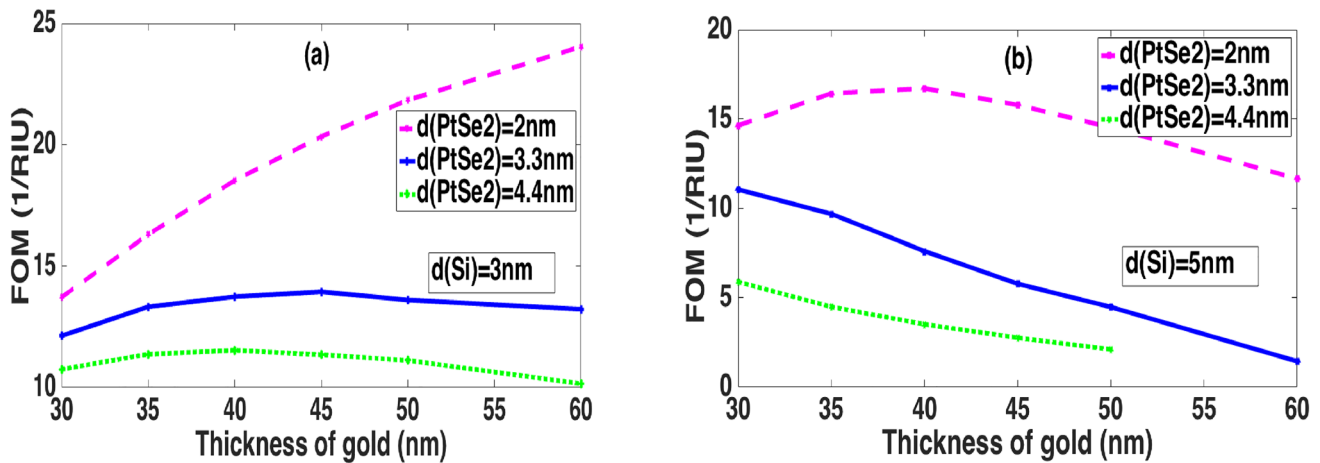


Fig. 6 The FOM as a function thickness of Gold $d(\text{Si}) = 3 \text{ nm}$ (a) and $d(\text{Si}) = 5 \text{ nm}$ (b)

Table 3 Comparison of proposed work with another existing sensor

| Ref | Enhancement strategy | | | | |
|------------------------|----------------------|----------------------|--------|-------------------------|--------------------------|
| | λ (nm) | S ($^{\circ}$ /RIU) | Rmin | QF (RIU ⁻¹) | FOM (RIU ⁻¹) |
| Xu et al. [40] | 633 | 156 | — | — | — |
| Srivastava et al. [41] | 633 | 190 | 0.0692 | 15.51 | — |
| Wu et al. [41] | 633 | 160 | — | — | — |
| Jia et al. [42] | 633 | 165 | 0.3515 | 14.12 | — |
| Rikta et al. [43] | 633 | 96.43 | — | 12.36 | — |
| Rahman et al. [31] | 633 | 200 | 0.2554 | — | 17.70 |
| kumar et al. [44] | 633 | 174.1 | — | — | — |
| Villarmi et al. [17] | 633 | 85.5 | — | — | — |
| Karki et al. [45] | 633 | 161 | — | 11.89 | 81.32 |
| Rahman et al. [30] | 633 | 194 | — | 34 | — |
| Proposed work | 633 | 200 | 0.0254 | 0.0822 | 16.43 |
| Proposed work | 633 | 206 | 0.6068 | 0.0815 | 24.03 |

It is expected that the novel structure may be very much useful in different fields of biosensing and optical sensing application.

Acknowledgements This work was funded by the Researchers Supporting Project Number (RSP2024R267) King Saud University, Riyadh, Saudi Arabia.

Authors contributions statements Conceptualization, Data curation: H. Bouandes. Formal analysis, Methodology: M.A. Ghebouli, M. Fatmi. Software: A. Djemli. Visualization, Validation, Writing—review & editing: Y. Slimani. Roles/Writing—original draft: K. Ayadi, M. Fatmi, Munirah D. Albaqami, Saikh Mohammad and Mika Sillanpaa, T. Chihhi.

Declaration

Conflict of interests The authors declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

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