Numerical design of high-performance WS$_2$/metal/WS$_2$/graphene heterostructure based surface plasmon resonance refractive index sensor

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ABSTRACT

The development of a high-performance bio-sensor utilizing the surface plasmon resonance (SPR) phenomenon has attracted great attention recently as a promising and precise sensing technology. Here, we proposed a WS$_2$/metal/WS$_2$/graphene heterostructure based SPR sensor with improved performances. The finite-difference time-domain (FDTD) technique was employed to model and develop the prospective sensor. The effects of integrating different layers, the analyte thickness on the performance of the sensor, and the electric field distribution were investigated systematically. We found that the optimized structure of the developed sensor exhibits the highest sensitivity of 208 deg/RIU with a detection accuracy of 1.12 and a quality factor of 223.66 RIU$^{-1}$, which is superior to existing two-dimensional material based SPR sensors. The enhancement of light-material interaction caused by the coating of a monolayer WS$_2$ on both sides of the metal improved the sensor performance significantly. These findings demonstrate a new way of performance enhancement in the composite layer sensor, aimed at further improving the identification of specific biomolecules such as glucose, blood disease, environmental monitoring, and agricultural applications.

Introduction

Of late, surface plasmon resonance (SPR) has appealed as one of the most promising sensing techniques due to its key benefits, including a high degree of sensitivity, more user-friendly, lower cost, as well as label-free and real-time identification over conventional biosensors. Such enticing features allow SPR-based sensors desirable for many biosensing applications, including temperature measurement [1], detection of formalin [2], human blood group [3], glucose [4], food and environmental interest [5], gas sensing [6], bacteria [7], urine [8], DNA hybridization [9], living cell analysis [10], etc. However, sensor performance is one of the vital aspects of biological sensing, and exploring the performance enhancement mechanism in SPR biosensors is a research hotspot. In an attempt to optimize the sensor performance, Shalabney et al. [11] suggested a variety of methods, such as optimization of metal layers, the effect of the prism index and dispersion, the addition of nano-dielectric layers, incorporation of the gratings on the top of metals. A bimetallic film was also suggested by Dyankov et al. [12] to enhance the sensitivity of the SPR sensor. In this regard, Kashyap et al. [13] and Chen et al. [14] proposed a bimetallic sensor based on Ag-Au with increased sensitivity and reduced FWHM compared to a single metal-based sensor, providing a high detection accuracy. Nevertheless, the performance of SPR sensors requires further enhancement for practical applications.

Thanks to their remarkable electrical and optical properties, two-dimensional (2D) materials such as graphene and transition metal dichalcogenides (TMDCs) have been used in recent years to build SPR sensors [15]. 2D materials have versatile biocompatibility and a greater adsorption surface area that improves sensor performance and quality [16]. TMDCs induce a strong coupling at the metal/TMDCs interface, which enhances the electric field. The enhanced electrical field is extremely sensitive to the analyte’s refractive index shift, resulting in improved sensitivity. Moreover, a larger real part of the dielectric constant of these materials enables the absorption of light energy by metal [17]. The sensitivity of the conventional SPR sensor is not high enough because the metal layer cannot absorb enough light energy for stronger excitation. However, TMDCs can absorb higher light energy due to its large real part of the dielectric constant, which provides stronger excitation. Besides, the metal layer can be covered by TMDCs, which offers better stability for the sensor. With these privileges, various SPR sensors

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have been proposed and investigated using 2D-materials. Wu et al. suggested an extremely sensitive SPR sensor based on graphene, which could improve the sensitivity by 25% [18]. A nanostructured SPR biosensor with enhanced sensitivity based on graphene-MoS$_2$ was suggested by Zeng et al. [19]. The TMDC/Silicon nano-sized SPR sensor was illustrated by Ouyang et al. [20]. They recorded the sensor’s optimum sensitivity was 155.68 deg/RIU with an FWHM of 17.46 deg. The efficiency of the sensor was also improved through black phosphorus (BP). Wu et al. [21] reported a biochemical sensor focused on the heterostructure of BP-graphene-bilayer-WSe$_2$ and enabled to attain the sensitivity of 279 deg/RIU. Although high sensitivity was achieved, however, the broadening of the SPR spectrum has not been shown. In the MoS$_2$-graphene-aluminum (Al)-based sensor, the sensitivity of 215 deg/RIU was also recorded when the analyte refractive index is 1.42 [22].

Moreover, recent investigations [22,23] show that the coating of different types of TMDCs on both surfaces of the metal film enhances the sensitivity greatly in the SPR sensor. A maximum sensitivity of 190 deg/RIU was obtained by coating MoS$_2$ on both surfaces of the metal film. A higher sensitivity of 215 deg/RIU was obtained for seven layers WSe$_2$, which is 3.3 times greater than the conventional Al thin-film based sensor. These studies suggest that graphene and TMDCs are excellent candidates for the sensitivity enhancement of the sensor.

Apart from the 2D materials, prior studies revealed that an introduction of an air gap could significantly enhance sensor performance. For instance, a graphene-based sensor with a high air gap of 23 nm has been proposed by Verma et al. [24] with sensitivity 2.35 times greater than that of without an air gap. Rouf et al. [25] proposed an Ag-Au bimetallic InP-based SPR biosensor with a 15 nm air gap, where they obtained the maximum sensitivity of 70.90 deg/RIU. Very high air gaps of 35 nm, 45 nm, and 55 nm have been proposed for graphene multilayer based SPR biosensor by Maharana et al. [26] with the sensitivity of 39.68 deg/RIU, 34.5 deg/RIU, and 33.42 deg/RIU for the wavelength of 700 nm, 850 nm, and 1000 nm, respectively.

Although the uses of TMDCs as well as the introduction of an air gap improve the sensitivity, the FWHM also increases in TMDCs based sensors, which reduces the sensor resolution. On the other hand, along with the large sensitivity, the narrow FWHM and quality factor (sensitivity/FWHM) are the important criteria to design the sensor with specific applications. To enhance the detection accuracy and quality factor, Bijalwan et al. [27] proposed a nanoribbon of graphene/WSe$_2$ structure. By optimizing the number of graphene and WSe$_2$ layers, they revealed that the detection accuracy and quality factor could be enhanced by 0.82 to 0.92 and 164.28 RIU$^{-1}$ to 184.97 RIU$^{-1}$ for graphene nanoribbons whereas 0.81 to 0.90 and 162.5 RIU$^{-1}$ to 181.11 RIU$^{-1}$ for WSe$_2$ nanoribbons, respectively. They also demonstrated that the FWHM increases with increasing layer numbers. However, increasing the layer numbers reduces the detection accuracy and quality factor. Thus, further research is essential to resolve how the sensor performance can be improved with the minimum TMDC/graphene layers.

In this work, with an intention to improve the sensitivity without costing the detection accuracy and quality factor, we proposed a WSe$_2$/metal/WSe$_2$/graphene heterostructure based SPR sensor. The Finite-difference time-domain (FDTD) technique was employed to model and develop the prospective sensor. Through enhancing light-matter interaction using a 2D WSe$_2$ layer on either side of the metals, the performance of the proposed sensor can be enhanced rather than by optimizing the thickness of the layer. The optimized design of the developed sensor revealed an angular sensitivity of 208 deg/RIU with detection accuracy 1.12 and quality factor 223.66 RIU$^{-1}$, which outperforms compared to the performance of any conventional configurations.

Materials and sensor design

The proposed SPR sensor is based on the Kretschmann configuration [28] using the heterostructure of 2D materials and thin metal layers. The angular interrogation method was applied to obtain the excitation of surface plasmon polarization (SPP). The p-polarized (TM) light with a wavelength of 633 nm was passed through different layers to obtain attenuated total reflection (ATR), which is reflected on the different layer interfaces and captured by the detector. For a particular incident angle, the wave vector is matched with the surface plasmon wave (SPW), known as SPR, and the corresponding angle is called the SPR angle. Consequently, minimal reflection occurs. Fig. 1 demonstrates the schematic of the proposed sensor. The basic structure of the developed sensor consists of 7th layers. The detailed specification and optimized parameters are illustrated in Table 1. We used CF$_2$ glass as a prism because the lower refractive index of prism offers high sensitivity [29]. The refractive index for CF$_2$ glass was determined using the following relation as [30]

$$\eta_{p_{\text{prism}}}^2 = 1 + \frac{0.5675888 \lambda^2}{\lambda^2 - 0.050263605^2} + \frac{0.4710914^2}{\lambda^2 - 0.1003909^2} + \frac{3.8484723^2}{\lambda^2 - 34.0649040^2}. \quad (1)$$

Aluminum (Al) was selected as an active metal due to its thinner SPR response. Al refractive index was determined employing the Drude equation as follows [31]:

$$\eta_{Al} = \left(1 - \frac{2 \pi^2 \omega_p^2}{\omega^2 + i \sigma} \right)^{1/2} \quad (2)$$

where $\lambda_p = 1.0657 \times 10^{-7}$ m and $\lambda_c = 2.4511 \times 10^{-5}$ m. A silver (Ag) layer was deposited on it since the use of a bimetallic structure enhances sensitivity in the SPR sensor highly [13,14]. Besides, Ag has the minimum FWHM [32], which increases the DA and QF. As our main concern in this work is the improvement of DA and QF with improving sensitivity, therefore, we have chosen Al/Ag instead of single plasmonic metal. However, Al and Ag both are chemically unstable and prone to oxidation. To stabilize the sensor, monolayer WSe$_2$ was placed on both sides of the metal so that metal can free from the chemical reaction and a huge amount of light energy can be absorbed. To further increase the sensitivity of the sensor, monolayer graphene was selected owing to its unique optical properties and exotic mechanical flexibility [33]. We determined the refractive index of graphene as [34]

$$\eta_G = 3.0 + \frac{i \sigma d}{3} \quad (3)$$

where $\epsilon = 5.446 \, \mu m^{-1}$.

All the simulations were performed by the 2D Finite-difference time-domain (FDTD) technique using the Numerical FDTD simulator (Version: 8.19,1584). Parameter sweep was conducted to attain the capability of the source angle to stimulate SPR mode. An overriding mesh area was taken to push a better mesh step size in the y-direction perpendicular to the metal film. The boundary condition was defined in such a way that the reflection of the outgoing wave was absorbed and inhibited. The most widely used absorbing boundary condition with extremely low local reflection is the perfectly matched layer (PML) [35,36]. The PML is a regime where the reflecting plane wave is polarized at a certain frequency and matches the boundary. The PML is intended to capture the outgoing wave from the active domain of computation without reflecting it back to the field of interest. To better absorb light propagating at broad angles from the usual incidence, the PML profile was set to a “steep angle” in this work.

Although this work proposed a numerical design of SPR sensor based on WSe$_2$/metal/WSe$_2$/graphene hybrid structure. However, our proposed theoretical design can also be experimentally realized. Al and Ag layer can be deposited with the help of the electron beam evaporation or sputtering techniques [37,38]. Graphene/WSe$_2$ can be deposited by the chemical vapor deposition (CVD) technique [39-42].

Performance parameters of the SPR sensor

The performance of the SPR sensor during assessment and sensing is...
indicated via various parameters. Sensitivity is considered as the main performance parameter, which can be obtained from the ratio of the SPR angle magnitude to the measurand or more specifically the refractive index. Usually, the angle at which minimum reflectivity occurs is indicated as an SPR angle. The slope of the standard graph is connected to this parameter. Generally, sensitivity (S) is formulated using the following relation [43].

\[
S = \frac{\Delta \theta_{\text{SPR}}}{\Delta \eta_a}; \text{deg/RIU} \tag{4}
\]

where \( \Delta \theta_{\text{SPR}} \) and \( \Delta \eta_a \) represent the change in SPR angle and refractive index of the analyte. The next performance parameter considered in this study is the detection accuracy (DA). This parameter is related to the full width at half maximum (FWHM) of the SPR sensor with the shifting of the SPR angle. The higher the DA, the better the SPR sensor. The DA is formulated as the change in the SPR angle with the spectral width at 50% reflectivity (i.e., FWHM) as [44].

\[
DA = \frac{\Delta \theta_{\text{SPR}}}{\text{FWHM}} \tag{5}
\]

Another crucial parameter used to characterize the performance of the proposed sensor is the quality factor (QF). The larger QF indicates the better performance of the sensor. The QF is calculated as the ratio of the sensitivity by the spectral width at 50% reflectivity as [23].

\[
QF = \frac{S}{\text{FWHM}} \text{RIU}^{-1} \tag{6}
\]

### Results and discussion

At first, we calculated the reflectivity for the various incidence angles generated by the angular integration technique with refractive index \( \eta_a = 1.33 \) and \( \eta_a = 1.335 \), considering a 633 nm TM polarized light at the prism-metal surface. Fig. 2a shows the reflection versus SPR angle characteristics of the CF$_2$/metal structure. The metal film dielectric constant has a significant impact on the SPR parameters. When polarized light strikes on the top of the plasmonic metal through a prism, the light is reflected by the metal film, which acts as a mirror. The polarized light can interact with the free electrons of metal films, generating an oscillation of electrons known as plasmon, thereby decreasing the intensity of the reflected light. For a particular incident angle, the incident light’s wave vector is equal to the surface plasmon wave (SPW), inducing an SPR excitation. The minimum reflection occurs at this angle, which is recognized as an SPR angle. Surface plasmon (SP) occurs at the interface of two materials where there is a different sign in the real part of the dielectric function. It is only possible in certain ranges of thickness of the metal film. The basic concept is that SPs are highly sensitive to any changes in the metal surface dielectric environment. Therefore, any slight variation in the refractive index causes a large variation in the SPR parameter. As a result, the SPR angle changes with the variation of the refractive index.

As Fig. 2a suggests, with the increase of the refractive index of the sensing medium, the SPR angle shifts to the right as well as the percentage of reflection increases. This phenomenon can be elucidated via the following relation [45]

\[
\theta_{\text{SPR}} = \sin^{-1} \frac{\eta_p \eta_a}{\eta_p^2 + \eta_a^2} \tag{7}
\]

here, \( \eta_p \) and \( \eta_a \) represent the refractive index of the CF$_2$ glass prism and the analyte, respectively. \( \eta_{\text{eff}} \) is the equivalent refractive index (RI) of
composite layers. From this equation, it is seen that the SPR angle depends on the $n_a$. Therefore, with an increasing refractive index of the analyte, the SPR angle is shifted to the right. The obtained SPR angles were 69.97 deg at $n_a = 1.33$ and 70.63 deg at $n_a = 1.335$. All the performance parameters of the sensor are proportional to the SPR shift. Due to the large shift of the SPR angle as well as the narrower FWHM (0.39 deg), the performance of the SPR sensor increases. The sensitivity, DA, and QF of the sensor were found as 132 deg/RIU, 1.69, and 338.46 RIU$^{-1}$, respectively. However, the sensitivity is not good enough and further improvement is required. Therefore, a monolayer WS$_2$ has been proposed to enhance sensor performance. Fig. 2b shows the sensor response curve after adding WS$_2$ monolayer on both sides of the metal. The SPR angle is changed from 75.13 deg to 76.07 deg, offering enhanced sensitivity (188 deg/RIU). However, the FWHM increases from 0.39 to 0.52 deg. Generally, the enhancing effect produced by WS$_2$ is associated with its dielectric constant. As can be perceived from Table 1, the WS$_2$ layer offers a higher real part of the dielectric constant, which provides a strong absorption ability [19,23], resulting in increased sensitivity. It can be explained by the following relation [19]

$$k_{sp} = \text{Re} \left[ k_0 \left( \frac{\varepsilon_{mw} n_a^2}{\varepsilon_{mw} + n_a^2} \right)^{1/2} \right]$$

(8)

where, $k_0$ is the wave vector of the incident light, $\varepsilon_{mw}$ is the dielectric constant of the WS$_2$ enhanced the metallic thin film, and $n_a$ is the refractive index of the analyte. According to Eq. (8), the SP wave vector ($k_{sp}$) increases due to a larger real part of the dielectric constant, resulting in a larger incident angle requirement for the SP excitation. Besides, $k_{sp}$ also increases with the increase of the analyte’s refractive index. Therefore, with a small increase of $n_a$ of the analyte, the value of $k_{sp}$ also increases, resulting in $k_{sp}$ is matched with $k_0$ at a larger incident angle leading to greater sensitivity. On the other hand, a large broadening is observed in the SPR curve due to the loss of electron energy related to the imaginary part of the dielectric constant [19]. Thus, to further improve the sensitivity, we selected a graphene layer on the WS$_2$ layer.

Fig. 2c shows the sensor response curve after adding the graphene layer. We observed that the SPR angle of 75.18 deg at $n_a = 1.33$ and 76.14 deg at $n_a = 1.335$, resulting in an SPR shift of 0.96 deg, which enhances the sensitivity to 192 deg/RIU. Similar to WS$_2$, graphene has also an imaginary part of the dielectric constant, which broadens the FWHM (0.61 deg). To further improve the performance, an air gap is introduced between the prism and WS$_2$ layer. Introducing an air gap, the sensor response curve is shown in Fig. 2d. The sensitivity, DA, and QF of the sensor were obtained as 208 deg/RIU, 1.12, and 223.66 RIU$^{-1}$, respectively, which is far better than the existing 2D materials based SPR sensors. Recent studies [23,27] show that the increasing number of TMDC and graphene layers provide better absorption, resulting in higher sensitivity with increasing FWHM due to higher electron energy loss. Nonetheless, the FWHM of the SPR reflection spectrum is also a crucial parameter along with the sensitivity that must be considered when designing a sensor. Thus, the impact of WS$_2$ and graphene layer numbers on sensor performance is ignored in this study.

To obtain the optimal thickness of different layers, especially the thickness of metal and air gap at which the maximum performance occurs, we have calculated the thickness dependence of the sensor performance. Considering the Ag layer thickness as 35 nm [23], we have optimized the thickness of the Ag layer and the air gap. Fig. 3a shows the sensitivity of the proposed sensor as a function of the Ag thickness without any air gap. The maximum sensitivity was found at the 20 nm thick Ag layer. A further increase in the Ag layer thickness reduces the sensitivity of the sensor, as shown in Fig. 3a. Assuming the optimized thickness of the Ag layer as 20 nm, the performance of the sensor as a function of the air gap thickness is presented in Fig. 3b. As Fig. 3b

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suggests, the highest sensitivity was achieved with an air gap thickness of 35 nm. The sensitivity starts to decrease as the air gap thickness increases more. Hence, the optimized thickness of the Ag and the air gap is determined as 20 nm and 35 nm, respectively.

To further analyze the sensor performance, the refractive index shift caused by the analyte is applied for a finite thickness. Under the optimized design condition, the sensor performance by varying the thickness of the analyte (50 nm-300 nm) is shown in Fig. 4. Although the sensitivity, DA, and QF all were found to increase with the increase in analyte thickness, the sensor still offers good performance at a lower analyte thickness. Even with a 50 nm thin analyte, the sensitivity, DA, and QF were still found to be as high as 26 deg/RIU, 0.43, and 86.67 RIU, respectively. The dynamic range of the proposed sensor was also analyzed. We have calculated the SPR angle for different refractive indices of the analyte which are plotted in Fig. 5. The angular response is observed to remain linear in the refractive index range of 1.33–1.36, indicating that any changes in this region can be detected.

For benchmarking, we also analyze the distribution of the electric field of the proposed sensor using the FDTD technique. A 633 nm plane wave TM polarized light source was considered to perform the calculation. Maxwell’s equation can be solved easily via the YEE algorithms in the FDTD, which makes it a versatile tool. Compared to other methods such as Green’s dynamic technique to resolve Maxwell’s equations for complex geometries and dispersive media [46], the FDTD technique provides more accurate results. The PML was used for boundary conditions to enable the waves to reach layers with minimal reflections (Rmin), and the electric field intensity was monitored using the DFT monitor. The distribution of the electric field in the proposed biosensor is depicted in Fig. 6. It can be perceived that the intensity of the electric field is different for different layers. The electric field strength reaches its optimum value if the reflectance curve shows the lowest reflectivity value. Maximum electric field intensity is obtained in the Al/WS2/graphene layer. It can be said that minimum reflection occurs in the metal layer in surface plasmon conditions. The incorporation of WS2 layers on the metal film induces a strong coupling at the metal/WS2 interface owing to the effective charge transfer. This effect greatly enhances the electric field at the sensing inter-face [47-52]. Consequently, an ultra-high sensitivity is perceived. Moreover, the use of WS2/graphene heterostructure increases the adsorption surface area due to van der Waals force of attraction and enhances the interface field, resulting in a further enhancement of sensitivity. In addition, the air gap in the proposed structure acts as a dielectric medium that increases the reflection spectrum’s resonance dip, resulting in an enhanced sensitivity. Besides, the probing field intensity decays exponentially to the analyte with a penetration depth of about 247 nm and the propagation length of about 198 nm. This indicates that the probing electric field near the sensing interface is very strong and would be highly sensitive to the interactions of small biomolecules.

A comparison has also been made between the proposed sensor and the existing 2D materials-based sensors. Table 2 represents the performances of the proposed sensor along with some existing 2D materials-based sensors designed in the earlier works. From the comparison table, it can be observed that the TMDC/graphene heterostructure-based sensor shows the highest sensitivity (315.52 deg/RIU) but very poor QF (18.84 RIU⁻¹). On the other hand, the sensor based on WSe2 and graphene nanoribbons improved the DA to 0.9 and 0.92 as well as the QF 181.11 RIU⁻¹ and 184.97 RIU⁻¹, respectively by the costing of sensitivity. This indicates that the overall performances of the reported sensors still need to be improved. On the other hand, the obtained performance (sensitivity = 208 deg/RIU, DA = 1.12, and QF = 223.66 RIU⁻¹) of the proposed sensor is much better than the existing 2D
In summary, we systematically modeled a WS$_2$/metal/WS$_2$/graphene heterostructure based SPR biosensor with improved performances employing the finite-difference time-domain (FDTD) technique. The effect of adding different layers, the thickness of the analyte on the sensor performance, and the electric field distribution have been investigated thoroughly to attain the optimal performance of the proposed sensor. The optimized structure of the designed sensor revealed a maximum detection accuracy of 1.12, a quality factor of 223.66 RIU$^{-1}$, and a sensitivity of 208 deg/RIU. The obtained performance is higher compared to the existing 2D materials based SPR sensor. The coating of a monolayer WS$_2$ on both sides of the metal enhances the light-matter-interaction greatly, which causes a significant improvement of the sensor performance. The proposed biosensor can be a promising candidate for high-performance bio-sensing in medical diagnostic, agricultural applications, and environmental detection.

### Conclusions

In summary, we systematically modeled a WS$_2$/metal/WS$_2$/graphene heterostructure based SPR biosensor with improved performances employing the finite-difference time-domain (FDTD) technique. The effect of adding different layers, the thickness of the analyte on the sensor performance, and the electric field distribution have been investigated thoroughly to attain the optimal performance of the proposed sensor. The optimized structure of the designed sensor revealed a maximum detection accuracy of 1.12, a quality factor of 223.66 RIU$^{-1}$, and a sensitivity of 208 deg/RIU. The obtained performance is higher compared to the existing 2D materials based SPR sensor. The coating of a monolayer WS$_2$ on both sides of the metal enhances the light-matter-interaction greatly, which causes a significant improvement of the sensor performance. The proposed biosensor can be a promising candidate for high-performance bio-sensing in medical diagnostic, agricultural applications, and environmental detection.

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### Data availability

The data that support the findings of this study are available from the corresponding author upon reasonable request.

### CRediT authorship contribution statement

**Biswajit Dey**: Conceptualization, Methodology, Software, Data curation. **Md. Sherajul Islam**: Writing - original draft, Visualization, Investigation, Supervision, Software, Validation. **Jeongwon Park**: Writing - review & editing.

### Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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