Optical biosensor based on enhanced surface plasmon resonance: theoretical optimization

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Abstract

In this article, a theoretical design of enhanced surface plasmon resonance is proposed. The suggested sensor is composed of titanium, silver, graphene, photonic crystal, and a sensing layer. This structure is used to detect cancer cells and hemoglobin in blood plasma based on their refractive indices. Different parameters such as sensitivity and figure of merit are studied at an operating wavelength of 633 nm. The recorded sensitivity and figure of merit are 72 degrees/RIU and 346 RIU⁻¹. The ability of the proposed sensor to detect cancer cells and blood plasma concentration will be investigated.

Keywords Plasmon resonance · Photonic crystals · Cancer cells · Sensitivity

1 Introduction

Surface Plasmon Resonance (SPR) is a collective oscillation of propagated free electrons at the interface between a metallic thin sheet and a dielectric layer (Choi et al. 2011; Balakrishnan et al. 2016; Singh et al. 2015; Singh and Black 2018). SPR is a physical effect that allows researchers to investigate real-time biomolecular interactions. This approach responds well to changes in the refractive index of the sensing material. This response happens as a result of changing the optical properties of the attached biomolecules to the surface (Foley et al. 2015; Kim 2010; Akimov 2018; Wu et al. 2016). SPR biosensors have been used in various applications such as plasmonic detectors, optical polarization encoding, sensing technology, and bio-photonic sensors (Dai et al. 2015; Xiang et al. 2014; Ooi et al. 2012; Singh et al. 2012; Esteban et al. 2011). Thin films of metals such as aluminum, gold, or silver can be utilized to determine molecular concentration for biosensing in conventional SPR (Homola 2008; Xinglong et al. 2003). The SPR angle is the angle

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of incidence in which minimum reflected light intensity happens between the metal and dielectric boundary.

There are different ways to enhance the performance of biosensors. Abdulhalim et al. improved the performance of the biosensor by combining a layer of high refractive index with the metallic sheet (Shalabney and Abdulhalim 2011; Lahav et al. 2008). Guerinik et al. introduced an $\text{Al}_x\text{Ga}_{1-x}\text{As}$ 70% Al on top of the gold/silver sheet as an SPR biosensor (Guerinik and Tayeboun 2020). Also, Chabot et al. manufactured a responsive sensor by utilizing SPR (Chabot et al. 2012). Recently, Graphene appeared as an excellent alternative to enhance biosensors' sensitivity because of its substantial adsorption property (Wu et al. 2010; Zaky and Aly 2021a, b; Liu et al. 2019; Zaky et al. 2021a). Graphene-on-silver design improved by a titanium layer (Ti) is employed for superior to prism glass adherence (Choi et al. 2011).

One-dimensional photonic crystals (1D-PhC) are periodic constructions in which the refractive index alters periodically through the structure (Zaky and Aly 2021c, 2020; Aly et al. 2021a, 2020; Zaky et al. 2020, 2021b). The refractive index of the sensing substance of the PhC or the defect layer can change the resonance wavelength (Prather et al. 2009; Aly et al. 2008, 2021b; Abd El-Ghany et al. 2020; Zaky et al. 2021c, d, e; Tammam et al. 2021). Hybrid configurations composed of two different structures of metal and photonic crystal (PhC) have also drawn much consideration in the latest times (Meradi et al. 2016; Sabra et al. 2018). Moradi et al. have described a susceptible sensor using a 1D-PhC with a sensitivity of 240 degrees/RIU (Meradi et al. 2016).

The present work reports a biosensor deposited on BK7 glass with a graphene-on-silver-titanium structure combined with a 1D-PhC to enhance the overall performance of the biosensor. This study assumes a 633 nm as a fixed wavelength, which is the typical emission wavelength of a He–Ne laser (Wu et al. 2016; Zeng et al. 2015; Sahu et al. 2009). The optimized structure is exploited for detecting the blood plasma and different cancer cells. Various cancer cells or blood plasmas located in analyte consequence in a displacement of the reflection ranges of our arrangements. The variation in the blood plasma's concentration or the cancer cells triggers a significant change to the resonant dips. Thus, by examining the suggested biosensor structures' reflectance spectra, it is feasible to calculate the various blood plasma concentrations and detect different cancer cells.

The novelty of this study is that a significant improvement is observed in the proposed biosensor's FoM compared with the conventionally reported biosensors, as clear in Table 3.

2 Description and analysis of the structure

The suggested SPR-PhC sensor is composed of titanium (Ti), silver (Ag), graphene, photonic crystals (PhCs), and sensing layer as clear in Fig. 1A. These materials are deposited on a BK7 glass prism with a refractive index RI of $n_1 = 1.515$ (Wu et al. 2017; Sreekanth et al. 2013). Ti layer has a refractive index of $2.7043 + i3.7657$ and a thickness of 1 nm (Johnson and Christy 1974). This layer of Ti is utilized to enhance the Ag layer's adherence to the optical prism glass (Choi et al. 2011). SPR sensor coated with Ag has better responsive than metals, however, silver is susceptible to oxidation. To avoid the oxidation of silver, Ag will be coated with a graphene layer. The refractive index of the Ag layer at the used wavelength is $0.059 + i4.243$ (Choi et al. 2011; Choi and Byun 2010), and its optimum thickness is 49.5 nm. The graphene's refractive index and thickness are respectively $n_G = 3.0 + i1.1491$ and $d_G = 0.34$ nm (Choi et al. 2011; Wu et al. 2017). A 1D-PhC structure contains N pairs of titanium dioxide-silica

Fig. 1 **A** Schematic diagram of suggested SPR-PhC multilayered configuration with N pairs of SiO_2 - TiO_2 layers, and **B** the configuration of SPR graphene-based sensor with titanium-silver

layers $(\text{SiO}_2 - \text{TiO}_2)^N$ with $n_{\text{SiO}_2} = 1.451$, $n_{\text{TiO}_2} = 2.232$ (Gao et al. 2012; Siefke et al. 2016), $d_{\text{SiO}_2} = \lambda/4n_{\text{SiO}_2}$ and $d_{\text{TiO}_2} = \lambda/4n_{\text{TiO}_2}$. Finally, we used water with a refractive index of 1.333 as a reference value for calibration. To compare our results, a conventional SPR structure will be studied as clear in Fig. 1B.

A monochromatic electromagnetic wave with wavelength $\lambda = 633$ nm propagates through the optical prism and is entirely reflected at the metal boundary creating an evanescent wave. The evanescent wave can penetrate the graphene and propagate along the x -axis with the wave vector constant of the following equation (Foley et al. 2015; Wu et al. 2016):

$$k_x = \frac{2\pi n_1}{\lambda} \sin\theta, \quad (1)$$

where θ is the incidence angle of the electromagnetic wave. The surface plasmon propagation constant k_{sp} is termed as (Foley et al. 2015):

$$k_{\text{sp}} = \frac{2\pi}{\lambda} \sqrt{\frac{n_m^2 n_t^2}{n_m^2 + n_t^2}}, \quad (2)$$

where n_m is the refractive index for the metal and n_t is the refractive index of the detecting sample material (n_t). SPR can be excited when the wave vector of the plasmon surface matches the wave vector of the incident electromagnetic wave. As a result, the incident electromagnetic wave resonantly couples with the plasmon surface, and a large enhancement of the electric field is realized with a minimum reflectance.

Studying the power of the reflected electromagnetic wave from an N -layer structure displayed in Fig. 1A for a TM electromagnetic wave polarization, the reflectance (R), is obtained by Guerink and Tayeboun (2020).

$$R = \left| \frac{(M_{11} + M_{12}q_N)q_1 - (M_{21} + M_{22}q_N)}{(M_{11} + M_{12}q_N)q_1 + (M_{21} + M_{22}q_N)} \right|^2, \quad (3)$$

$$M_{ij} = \left(\prod_{k=2}^{N-1} M_k \right)_{ij} \quad i, j = 1, 2, \quad (4)$$

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

$$q_k = \frac{\sqrt{\epsilon_k - n_1^2 \sin^2 \theta}}{\epsilon_k}, \quad (6)$$

$$\beta_k = d_k \left(\frac{2\pi}{\lambda} \right) \sqrt{\epsilon_k - n_1^2 \sin^2 \theta}. \quad (7)$$

The k_{th} layer has an electric permittivity (ϵ_k) and thickness (d_k), where k is from 2 up to $N-1$. Numerous factors are utilized to evaluate the performance of an SPR sensor. The fraction of shift of the resonance angle ($\Delta\theta_{sp}$) to the change in the analyte refractive index (Δn_i) is defined as sensitivity (S) (Verma et al. 2011):

$$S = \frac{\Delta\theta_{sp}}{\Delta n_i} (\text{degree/RIU}). \quad (8)$$

However, another critical parameter for evaluating is the figure of merit (FOM) (Meshginqalam and Barvestani 2018):

$$FOM = \frac{S}{FWHM} (\text{RIU}^{-1}), \quad (9)$$

where FWHM is the full-width at half maximum of the resonant dip. To improve the SPR sensor's resolution, it is required to reduce the FWHM of the reflectance dips to reduce the ambiguity in the resonance dip's fixation.

3 Results and discussions

The SPR excitation is a result of the total internal reflection (TIR). The TIR of reflectance spectra of SPR-PhC structure at $N=6$ takes place at the critical angles $\theta_c \sim 69.95^\circ$ for $n_i = 1.423$ and $\theta_c \sim 61.65^\circ$ for $n_i = 1.333$, as clear in Fig. 2A. The θ_c value is associated with the refractive index of the prism corresponding values (n_i) and the refractive index of the analyte (n_i). The SPR occurs at angles $\theta_{sp} = 71.55^\circ$ and $\theta_{sp} = 74.24^\circ$ for $n_i = 1.333$ and $n_i = 1.423$, respectively, as clear in Fig. 2A.

Figure 2B shows the reflectance spectra of the conventional SPR. TIR takes place at the critical angle ($\theta_c \sim 69.99^\circ$ for $n_i = 1.423$ and $\theta_c \sim 61.64^\circ$ for $n_i = 1.333$). The minimum reflected intensity confirms the excitation of the SPR. For the conventional SPR, the resonance is obtained at angles $\theta_{sp} = 68.23^\circ$ and $\theta_{sp} = 85.21^\circ$ for the water-sensing layers with $n_i = 1.333$ and $n_i = 1.423$, respectively.

The SPR-PhC structure recorded sensitivity of 29.9 degrees/RIU and FoM of 83.7 RIU⁻¹. On the other hand, the conventional SPR structure recorded a sensitivity of 188.5 degrees/RIU and FoM of 119.6 RIU⁻¹. From the first study, the SPR-PhC structure

Fig. 2 The reflectance of the **A** SPR-PhC structure at $N=6$, **B** conventional SPR structure as a function of the incidence angle for different analyte refractive indices

beats the conventional SPR structure in terms of the FWHM, but the conventional SPR structure beats in terms of sensitivity and FoM. In the following study, the geometrical parameters of the SPR-PhC structure will be optimized to achieve the highest performance with the lowest FWHM.

Because optimizing the geometrical parameters of the SPR-PhC structure will improve the sensitivity of SPR, the number of periods and the thickness of the PhC layers will be studied at different values. According to the reflectance spectra in Fig. 3A, by increasing the number of periods from 4 to 9, the width of the dips decreases. As clear in Fig. 3B, the structure records the highest sensitivity and high FoM at $N=4$ and will be the optimum condition.

Figure 4 illustrates the performance of SPR-PhC for different thicknesses of PhC layers ($\text{SiO}_2\text{-TiO}_2$) by changing n_t from 1.333 to 1.423. The sensitivity and FoM of the model are calculated when a beam of light with a wavelength of 633 nm is incident into it. In Fig. 4, the maximum sensitivity and FoM were recorded to be as high as 73.7 deg/RIU and 196 RIU^{-1} at an optimal thickness of $0.4 \cdot d$. For lower values than $0.4 \cdot d$, the resonant dips disappear. The optimized structure consists of a prism BK7, Ti, Ag, graphene, and four pairs of $\text{SiO}_2\text{-TiO}_2$ layers. The remaining parameters are the same as those in Fig. 1A, while the thicknesses of each layer in the PhC $\text{SiO}_2\text{-TiO}_2$ are respectively, $d_{\text{SiO}_2} = 0.4 \cdot \lambda / 4 \cdot n_{\text{SiO}_2}$, $d_{\text{TiO}_2} = 0.4 \cdot \lambda / 4 \cdot n_{\text{TiO}_2}$.

Fig. 3 **A** The reflectance of the SPR-PhC structure at $n_t = 1.333$ as a function of the incidence angle for a different number of periods, and **B** sensitivity and FoM of the sensor at different N by changing n_t from 1.333 to 1.423

Fig. 4 The sensitivity and FoM of the sensor at $N=4$ for different thicknesses of PhC layers by changing n_t from 1.333 to 1.423

Because some biofluids such as hemoglobin, blood glucose, and cancer cells have their refractive indices spread over n_t values between 1.3 and 1.42 (El-Khozondar et al. 2019; Aly and Zaky 2019; Ramanujam et al. 2019; Bijalwan and Rastogi 2018), we will focus the numerical simulations on this range. This allows us to say that our proposed sensor can be used for bio-detection. To justify this choice, we have analyzed our sensor's performance for the blood plasma cell and cancer detection application. The refractive indices of the various blood plasma cells are taken from reference (El-Khozondar et al. 2019). As clear in Table 1, the refractive index of blood plasma can be calculated as a function of plasma concentration (C_p) as the following (El-Khozondar et al. 2019):

$$n_t = 1.32459 + 0.001942C_p \quad (10)$$

We can see that the resonance angle moves towards higher angles as much as the plasma concentration increases because the refractive index of the blood changes as much as the concentration changes as clear in Fig. 5.

The sensitivity of this bio-sensor increases by increasing the plasma concentrations. Besides, the FoM of the proposed structure is very high. The calculated parameters describe the potential of the proposed sensor for different concentrations of the blood plasma cell, particularly the most concentrated. The calculated highest sensitivity of the sensor is 72 deg/RIU with a FoM of 345.8 RIU⁻¹ (Table 2).

We have also used this structure to detect cancer cells. Figure 6 illustrates the different reflectance spectra for different angles of incidence for various cancer and healthy cells (zero cancer), which are considered reference samples. We observe that θ_{sp} changes when different cells are present. The highest sensitivity is 71.5 deg/RIU with a FoM of 271.5 RIU⁻¹. These results describe the potential of the proposed sensor to sense blood plasma and different

Table 1 The sensitivity and FoM of the proposed sensor for different concentrations of blood plasma

Blood plasma	Refractive index (n_t)	Sensitivity (deg/RIU)	FoM (RIU ⁻¹)
0 g/L	1.32459	—	—
10 g/L	1.34401	58.3	161.4
20 g/L	1.36343	61.1	183.1
30 g/L	1.38285	64.1	213.0
40 g/L	1.40227	67.7	259.9
50 g/L	1.42169	72.0	345.8

Fig. 5 The reflectance of the SPR-PhC structure as a function of the incidence angle for a different concentration of blood plasma values at a thickness of each layer in the PhC = $0.4 \times d$

Table 2 The sensitivity and figure of merit of the sensor for different cancer cells (Aly and Zaky 2019; Ramanujam et al. 2019):

Cells	n_t	Sensitivity (deg/RIU)	FoM (RIU ⁻¹)
Normal cell	1.350	—	—
Jurkat cell	1.390	69.3	241.1
Hela cell	1.392	69.7	246.1
PC12 cell	1.395	70.3	253.9
MDA-MB-231	1.399	71.1	265.3
MCF-7 cell	1.401	71.5	271.5

Fig. 6 The reflectance of the SPR-PhC structure as a function of the incidence angle for different cancer cells at a thickness of each layer in the PhC = $0.4 \times d$

cancer cells. Finally, we can say that the performance of the proposed structure for detecting blood plasma is higher than the performance for cancer cell detection.

Based upon this investigation, we obtain a considerable sensitivity of 73.7 deg/RIU and FoM of 346 RIU⁻¹, as clear in Table 3. A significant improvement is observed in the proposed biosensor's FoM compared with the conventionally reported biosensors.

Table 3 Comparison of different performance parameters of the suggested SPR-PhC with other reported SPR biosensors

References	Sensitivity (degree/RIU)	FoM (RIU ⁻¹)
Kushwaha et al. (2018)	101.6	15.1
Rahman et al. (2017a)	80.7	–
Maurya and Prajapati (2016)	64.4	184.0
Rahman et al. (2017b)	87.8	–
Ouyang et al. (2016)	~ 126.0	~ 6.4
Verma et al. (2015)	68.0	–
Rahman et al. (2020)	94.3	–
Our work	72	346

4 Conclusion

In these simulations, a novel design achieved a much sharper SPR compared to other structures. Besides, it can have a high sensitivity and FoM. The proposed configuration provides an innovative idea of using the enhanced SPR-PhC structure to excite plasmonic modes. Further, the applications of this structure as blood plasma and cancer cell sensors were studied. The highest sensitivity is 72.0 deg/RIU with a FoM of 345.8 RIU⁻¹ and 71.5 deg/RIU with a FoM of 271.5 RIU⁻¹ for blood plasma and cancer cells sensor, respectively. The sensitivity of this bio-sensor increases by increasing the plasma concentrations. The optimizations of different parameters are done by using the TMM code. Besides, the FoM of the proposed structure is very high. These results cleared the proposed biosensor's potential for sensing the different blood plasma concentrations and various cancer cells.

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Declarations

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