Highly sensitive silicon nitride biomedical sensor using plasmonic grating and ZnO layer

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Abstract
A biomedical sensor that sense concentration of glycerol in a deionized water with a high sensitivity is introduced in this work. A silicon nitride layer is added to the grated substrate, glass, then a plasmonic layer has been used before adding a zinc oxide layer on the top of the plasmonic gratings. The dimensions of all layers have been optimized to obtain the maximum refractive index sensitivity. Finite difference time domain method is used to calculate a transmitted signal from the proposed structure with and without analyte material. Figure of merit, quality factor and full width half maximum are also calculated at different duty cycle. The best performance of the sensor has been obtained at duty cycle 35%, figure of merit 57.6, quality factor 57.3 and linewidth 14 nm. The maximum refractive index sensitivity is 806 nm/RIU which calculated at the same duty cycle. Detecting the glycerol concentration in deionized water is simulated at the maximum sensitivity and measured at different incident light angle. Finally, electric and magnetic fields and optical power, distributed along the structure are illustrated and discussed.

1. Introduction
Label free, quick response, high sensitivity and its compactness on a chip are the main advantages of a nanophotonic resonant used as biosensors [1–3]. Most of nanophotonic biosensors sense the change in the refractive index in the surrounding medium when the binding process of molecules or analyte is occurred [4]. The transmitted wavelength of the incident optical signal from the nanophotonic structure is shifted according to the surrounding refractive index change. The peak wavelength shift is depending on the change in the refractive index of the binding molecules which determines the refractive index sensitivity of the biosensor [5].

In order to fabricate a high sensitive biomedical sensor, some materials can be used such as, Silicon Nitride, Si$_3$N$_4$, which is considered as one of the efficient materials used in biosensors. It has some advantages over other materials such as, its integration of compacting, an ability to confine high optical power and low scattering loss from its sidewall roughness [6–8]. Si$_3$N$_4$ is a transparent material and can be fabricated using deposition technology which used as a waveguide grating coupler and high efficient biosensors [9]. On the other hand, titanium oxide material, TiO$_2$, is much better to use in biosensors for its transparency, wide band gap, low absorption loss in the visible region [10]. However, in this work, the Si$_3$N$_4$ material has been chosen for its efficient petperities in the visible and near infra red region and integration with CMOS technology which required high absorption in both regions. Recently, Zinc Oxide, ZnO, is used in biomedical sensors technology for its high performance such as high electron communication, nontoxic and high isoelectric point which allow a substance with low isoelectric point to attach on its surface and immobilize them to their biological activity after the binding process which in not the case when using gold material [11–13]. For this resone, it is used in the biosensor applications to enhance its performance [14].

A high sensitive biosensor is introduced in this work, which benefits from the advantages of using Si$_3$N$_4$, ZnO and plasmonic gratings materials. There are some related recent works were done in order to introduce a high-sensitive biosensor as illustrated below.
Abdul Shakoor and *et al* introduced a one-dimensional Si$_3$N$_4$ grating structure used as a biosensor with an experimental refractive index sensitivity reaches to 160 nm/RIU with linewidth 8 nm [15]. The sensor is suitable with a complementary metal oxide semiconductor (CMOS) detectors and can distinguish bio-species like DNA or protein. A high-contrast grating based on silicon structure is produced by T. Sun and *et al* [16]. The reported refractive index sensitivity was 418 nm/RIU, the quality factor was 3000 and the linewidth was 0.5 nm when using a tunable laser source centered at 1550 nm. A finite difference time domain (FDTD) simulation of a nanograting based a thin gold film using Fano resonances has been provided by Beibei Zeng and *et al* [17]. The deleted resolution of the provided structure is simulated and found to be 1.46 $\times$ 10$^{-6}$ RIU at a Temporal resolution of one second for a structure dimension 50 $\times$ 50 $\mu$m$^2$. A high sensitive Mach–Zehnder Interferometer, MZI, biosensor is introduced by Manolis and *et al* [18]. A plasmonic strip is designed in the sensing arm and optical anttenuator is incorporated in the reference Si$_3$N$_4$ arm to produce a 1930 nm/RIU refractive index sensitivity. TiO$_2$ material is also used as a high sensitive biomedical sensor by Sharma and Pandey [19]. They produced a plasmonic sensor with a sensitivity of 693.88 nm/RIU in the optical communication band. TiO$_2$ grating placed on an Au thin film material on a top of silica substrate has been analyzed using a broad range of analyte reflective indices. Three oxide layers has been added to a fiber optic to enhance the sensitivity, more than 3000 nm/RIU, as given by Singh and *et al* [20]. The used oxide layers are TiO$_2$, SiO$_2$ and SnO$_2$ which added on a top of copper layer and placed on an optical fiber side. However the introduced sensors is not compatible with CMOS devices as tiped on the optical fiber surface.

In this work, a ZnO layer based on a plasmonic grading and silicon nitride layer structure is designed and used to detect analyte (water and glycerol) in a visible or near infra-red regions. The introduced biosensor has advantages of using plasmonics materials, ZnO and Si$_3$N$_4$ to produce a high refractive index sensitivity. Compared to the related work, which gives a low sensitivity or not compatible with CMOS devices, the given sensor has a high sensitivity, 806 nm/RIU, and integrated with COMS devices. The proposed structure is simulated and analysed using FDTD Lumerical simulation tool. The shifting in the SPR peak wavelength is based on the change of the surrounding refractive index and the sensitivity is calculated based on the shifted wavelength. The optimization process of Si$_3$N$_4$ grating structure and ZnO plasmonic layers thickness will be also introduced.

### 2. Proposed structure and analysis method

The proposed structure will sense the concentration change of glycerol in a deionized (DI) water, which is represented by refractive index change (ranging from 1.333 for a pure DI water, to 1.474 for 100% glycerol in a DI water) [21]. The shift in the peak wavelength reflects the refractive index change on the top of the introduced structure according to the concentration of the binding glycerol in a DI water.

The proposed biosensor structure is illustrated in figure 1, where $P$ and $w$ are the grating period and grating width, respectively. Plasmonic and ZnO thicknesses are $x_1$ and $x_2$, respectively, $d$ is the grating depth and silicon nitride thickness is $t$.

In the given design, a periodic structure is considered in both sides of the sensor $x$- and $y$- coordinates and as a perfect matched layer in $z$-dimension that used as absorbing boundary condition. The simulation tool is an electromagnetic (EM) wave solver, which analyse the EM waves inside and outside the sensor. The modulated permittivity in the grating region is calculated using Fourier expansion shows in equation (1) [22].
where $\varepsilon_m$ is the $m$th Fourier component of relative permittivity in the grating region. And hence, the peak wavelength, $\lambda_{\text{peak}}$, can be determined using equation (2) [5].

$$\lambda_{\text{peak}} = \frac{P}{q} \sqrt{\frac{\varepsilon_{\text{med}}\varepsilon_0(\lambda_{\text{peak}})}{\varepsilon_{\text{med}} + \varepsilon_0(\lambda_{\text{peak}})}}$$

where $q$ is an integer, $\varepsilon_{\text{med}}$ is the permittivity of the surrounding medium, and $\varepsilon_0$ is the gold grating permittivity. The refractive index sensitivity, $S_n$, is considered the main sensor parameter and can be defined as a ratio between the change in the resonance wavelength, $\Delta \lambda$, to the change in the refractive index contacting medium, $\Delta n$, as

$$S_n = \frac{1}{\lambda_{\text{peak}}} \frac{\Delta \lambda}{\Delta n}$$
illustrated in equation (3).

\[ S_n = \frac{\delta \lambda}{\delta n} \text{ (nm/RIU)} \]  

(3)

where RIU is the refractive index unit [23].

Also, figure of Merit, FOM, is a very important parameter that indicates the performance of a biosensor. Figure of merit is defined as a ratio between a refractive index sensitivity and the Full Width Half Maximum, FWHM, \( \Delta \lambda \) as shown in equation (4) [24].

\[ \text{Figure of Merit} = \frac{S_n}{\delta \lambda \text{ (at FWHM)}} \]  

(4)
Finally, the Quality factor, Q-factor, is an indicator of the biosensor quality, and can be calculated using equation (5) [25].

\[
Q\text{-factor} = \frac{\lambda_{\text{peak}}}{\delta \lambda \text{ (at FWHM)}}
\]  

(5)

The transmitted electromagnetic signal is calculated by solving Maxwell’s equations around and inside the proposed sensor using FDTD method.

A backward incident light, plane wave Bloch/periodic, is used as a light source and the transmitted signal through the surface is received on the other side on the structure, as illustrated in figure 1. The peak wavelength of the transmitted signal is shifted according to the sensing glycerol concentration. Based on this shift, the refractive index sensitivity, figure of merit and quality factor are calculated. The optimum dimensions of a Si3N4, gold nanograting and ZnO layers are optimized in the following section. The effect of changing the grating period and duty cycle on the sensitivity, FOM and Q-factor is calculated and illustrated in the following section. Finally, the transmitted signal, for different glycerol concentration and changing the incident angle, is also studied and given in the results section.

3. Results and discussion

A unit cell with a period P has been simulated which is periodic in both x- and y- directions and PML in the z-direction. In the simulation setup, a 2D simulation in both x- and z- directions has been considered as there is no change in y- direction.

3.1. Grating design

The basic structure of the biosensor is the periodic gratings substrate with period P, 550 nm, and height d, and Si3N4 layer of height t. In order to obtain the maximum refractive index sensitivity, \( S_n \), a wide range of the height \( d \) and thickness \( t \) are tested. Figure 2 shows the sensitivity for the grating height ranging from 100 to 300 nm and silicon nitride thickness, \( t \), ranging from 100 to 300 nm. The maximum refractive index sensitivity, \( S_n \) = 228 nm/RIU, is obtained at \( d = 200 \) nm and \( t = 150 \) nm.

Then, a plasmonic gold layer and a zinc oxide layer have been added to enhance the sensitivity of the sensor. The sensitivity at different plasmonic thickness, \( x_1 \), ranging from 20 nm to 120 nm and ZnO thickness, \( x_2 \), ranging from zero, no ZnO layer, to 40 nm are simulated and illustrated in figure 3. In case of no ZnO layer, the sensitivity is very low, 266 nm/RIU at 100 nm Au thickness. The maximum sensitivity, \( S_n = 442 \) nm/RIU, is given at a plasmonic thickness \( x_1 = 100 \) nm and zinc oxide thickness \( x_2 = 20 \) nm, Red curve in figure 3.

Hence, the optimum grating dimensions are optimized as, \( d = 200 \) nm, \( t = 150 \) nm, \( x_1 = 100 \) nm and \( x_2 = 20 \) nm and the maximum sensitivity is 442 nm/RIU. The calculated values are obtained at a period grating with period \( P = 550 \) nm and duty cycle 0.5, where the duty cycle is the ratio between the width and the period of the unit cell, Duty cycle = \( \frac{W}{P} \).

3.2. Effect of changing duty cycle

The structural duty cycle is the main factor that affecting not only the sensitivity but also FOM, Q-factor and the linewidth. Figure 4(a) illustrates the refractive index sensitivity as a function duty cycle, 25%–75% with 5% step, which
gives a high sensitivity, 806 nm/RIU, at 35% duty cycle. A high FOM is also obtained at 35% duty cycle, 57.6, as given in figure 4(b). FOM is also changed with the duty cycle and clearly shown in figure 4(b), FOM decreases as the duty cycle increases due to the decreasing of the plasmonic and ZnO area with respect the substrate grating. As the sensitivity and FWHM are changed with changing the duty cycle, the FOM and Q-factor are also follows the same trend as expected from equations (4) and (5). Also, the maximum value of the quality factor can be noticed in figure 4(c), at duty cycle 35%, and its value is 57.3. Finally, the full width half maximum is 14 nm at the same duty cycle as shown in figure 4(d), which is a narrow linewidth.

So, the best performance of the given biosensor can be obtained at duty cycle 35% which gives the maximum FOM, Q-factor and a very low FWHM.

3.3. Detecting glycerol concentration and the incident light angle
To detect the glycerol concentration in a deionized water, we need the refractive index of each glycerol concentrations. Table 1 shows different glycerol concentrations and its associated refractive index [21].

![Figure 7](image-url) Distribution of (a) power (b) electric and (c) magnetic fields along the structure.
Hence, the shifting in the transmission spectrum for each concentration can be simulated at a duty cycle 35% which gives the maximum sensitivity, $S_n = 806 \text{ nm/RIU}$. Figure 5 shows the shifting in the wavelength due to the changing in the glycerol concentration, pure DI water, 20%, 40%, 60%, 80% and 100% glycerol.

The transmission spectrum can also be introduced as a function of the angle of the incident light, as illustrated in figure 6.

The incident angles have been changed from $0^\circ$ to $80^\circ$, with a step of $10^\circ$, and the spectrum of the transmitted signal is also changed accordingly. The transmission intensity decreases as the incident angle increases in the mid-band, 0.8–1.2 nm, however the angles between $10^\circ$ to $30^\circ$ have up normal behaviour in this region and have high transmission intensity in the visible region.

### 3.4. Electric and magnetic fields and optical power distribution

The electromagnetic optical power distributed along the structure is shown in figure 7(a), where most of the power is transmitted through the gratings, shown as a blue colour in the figure. Figure 7(a) shows that, the signal power is transmitted through the gratings, Au and ZnO, and absorbed at the non-grating areas. The transmitted power through Au and ZnO layers depends on the surrounding medium, analyte, and hence, the shift in the received signal wavelength is noticed at the monitor side. On the other hand, almost all electric field is transmitted out of the sensor as shown in figure 7(b). The magnetic field is also given in figure 7(c), which illustrate that, the magnetic field is transmitted through the gratings and affected by the analyte material as a surrounding medium.

A high refractive index sensitivity has been obtained from the introduced biomedical sensor, 806 nm/RIU, which is much higher than other models when sensing analyte material. The comparison is illustrated in table 2, between the proposed and other models.

In the detection process, the proposed sensor detects one concentration at a time, the complex concentration samples are not considered.

### 4. Conclusion

A high-performance biomedical sensor able to detect glycerol concentration in deionized water has been introduced and analysed in this work. The structural dimensions have been determined to obtain the maximum refractive index sensitivity, before adding plasmonic and zinc oxide layers. The calculated sensitivity at this stage was 442 nm/RIU. Then FOM, Q-factor, FWHM and sensitivity are calculated at differed duty cycle to maximize the biosensor performance. The maximum obtained sensitivity is 806 nm/RIU, FOM 57.6, Q-factor 57.3 and FWHM 14 nm at duty cycle 35% which is a very high-performance sensor compared to the other sensors mentioned in the literature. The transmission spectrum for different glycerol concentration is also produced for DI water, 20%, 40%, 60%, 80% and 100% concentration. Also, the angle of the incident light is changed from $0^\circ$ to $80^\circ$ with $10^\circ$ step and the intensity of the transmitted light is measured accordingly. Hence, it is easy to notice that, the chang in incident angle will not affect the resonance location but the intensity of the transmitted signal. Finally, distribution of the electric and magnetic fields and the optical power are also illustrated in this work.

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