Sensitivity Analysis Of Metasurface Array-Based Refractive Index Biosensors

Shobhit K. Patel, Juveriya Parmar, Rozalina Zakaria, Sharafali A, Truong Khang Nguyen, and Vigneswaran Dhasarathan

Abstract—This work intends for sensitivity analysis of different metasurface array-based biosensors. The array designs in the form of circle array, square array, square circle array, circle square array, five-element square array, plus array, five-element plus square array. The sensitivity of these metasurface biosensors are compared and optimized design is presented. Circle array design shows the best sensitivity performance amongst them. The optimized circle array design is analyzed by varying different physical parameters of the design such as SiO$_2$ substrate thickness and metasurface array thickness. The optimized results for this variation are also presented. The sensitivity of the current biosensor design is also compared with the previously published similar designs. The results are also presented for electric field intensity and current field density for the optimized design. The proposed sensitive biosensor can become a building block of future biomedical devices and photovoltaic devices.

Index Terms— Sensor, refractive index, graphene, metasurface, sensitivity.

I. INTRODUCTION

Biosensors are important in sensing biomolecules applicable in medical and photovoltaic applications. Biosensors are connecting biological components on surface of transducer which generates electric signals for detection. Optical biosensor used widely among the other type of biosensors due to its change in optical properties such as absorption, reflection, etc. In optical biosensors, change in signal of photodetector is converted to electric signal [1-2]. Optical biosensor receives an immense response in surface plasmon resonance for detecting molecular interaction, its usage covers every stage required for drug discovery in both academic and industrial fields. Surface plasmon resonance biosensor is the attraction in the field of biology helpful in the medical and environmental fields that are used for the detection of chemical and biological components [3-4]. The pathogenic microorganism that is responsible for dangerous diseases can be detected using optical biosensor that is helpful to environment and saves them from many disaster causes [5]. Silicon material is generally used while designing biosensor using integrated optics(IO) which is a part of photonics used for sensing as it is cost effective[6]. Silicon-based photonic sensor is used to improve sensitivity with the cost range that can be used for the detection of viral diseases such as cancer [7]. Optical biosensor mainly uses refractive change as a sensing tool, simulations and experiments are mainly based on the refractive index. They use label-free detection protocol for designing biosensors in which unrecognizable biomolecule can also be determined [8]. Photonics biosensor used due to its fabrications is compact and easy with less cost and wide applications in the field of medicine, environment, defence, etc [9].

The sensitivity is very important in designing any biosensor. This sensitivity is improved by incorporating graphene in the biosensing materials. Graphene has excellent electrical and optical properties which help in achieving higher sensitivity. Graphene made sensors and biosensors are much in demand due to their electrochemical properties that are useful in increasing sensitivity [10-11].Graphene oxide with its elasticity and flexibility is easy to combine with the substrate that has an impact on fabrication and it also helps in improving the characteristic of biosensing [12]. Graphene-based optical sensors are used to determine biomolecular interaction and observe movement in the structure that are useful in increasing sensitivities and accuracy in detection [13]. Graphene perturbation used in silicon nitride waveguide increases the sensitivity which is helpful in health applications [14]. SPR biosensor using graphene sensing layer fabricated on the gold thin film enhances the sensing of biosensor [15]. Graphene-based biosensors are used for sensing DNA. Graphene-based biosensors can also be used for environment analysis [16]. The graphene-based grating can be used to enhance the absorption using graphene-silica hybrid structure [17]. Hybrid nanocomposite glucose sensor made by combining nanocomposite material with graphene can be used for clinical applications [18].

Refractive index change biosensors are gaining interest among the researchers because of its narrowband response and higher sensitivity [19-24]. The change in refractive index increases the sensitivity by attenuated total reflection (ATR) method [19]. The 2,4,6 trinitrotoluene(TNT) can be detected using graphene oxide with label-free optical biosensor from...
which absorption response of biomolecule can be observed clearly in presence of TNT that is useful in sensing [20]. Early detection of cancer disease is possible using refractive index biosensor [21]. Refractive index biosensor is also used to design broadband and tunable spectrum [22-24].

The importance of using metasurface in changing surface wave phenomenon is explained [25-26]. The plasmonic phenomenon and its importance in sensing medium is presented in [27]. The use of nanoparticles with metasurface helps in improvement in many design parameters. This improvement in parameters can be used to improve the sensing of biomolecules [28-29]. The metasurface biosensing can be applicable in absorbers, medical applications, environment applications, automotive applications, etc [3-4, 30]. The experimental reports on fabricating biosensors for sensing hemoglobin biomolecules are presented in [31-33].

The design of biosensors is important because of its sensitivity and its spectrum. There is a need for a sensitive biosensor with simple design that can be used easily in medical applications. Here we have proposed different simple metasurface array biosensors and analyzed it for its sensitivity. We have provided its sensitivity analysis and also optimized the design by comparing all the designs. The optimized design is also compared with previously published designs to show its improvement. The biosensor designs and its design analysis is presented in Section II. The results of all the biosensor designs, its comparison, and optimized design are presented in Section III. The conclusion in terms of sensitivity and optimized design is presented in Section IV.

II. BIOSENSORS DESIGN AND ANALYSIS

The designing of biosensor is very essential because the proper design gives higher sensitivity which is required to sense the biomolecules. We have designed graphene-based metasurface biosensor for different metasurface combinations. The detailed design of the biosensor with all the metasurface combinations is presented in Fig. 1 and Fig. 2. The analysis of biosensor is presented in equation (1-12) for its sensitivity analysis, metasurface analysis, reflection, and absorption analysis.

The metasurface array-based biosensor is presented in Fig. 1. The 3×3 array of gold circular disks are used as metasurface elements in this biosensor design. The thickness of this gold circular disks is 0.3 μm thick and diameter of these circular disks is 0.5μm. These metasurface elements are placed above a thin graphene monolayer with its thickness of 0.34 nm. The graphene layer is placed on SiO₂ layer with its thickness 0.5 μm. The total structure area is 2.5×2.5 μm². The biomolecules are placed above gold metasurface elements and thickness of biomolecules layer is kept 0.6 μm.

We have changed these gold metasurface elements shapes to check its effect on the sensitivity of the biosensor. We have shown the seven different metasurface array elements used for biosensing in Fig. 2. The seven different metasurface designs are circle array, square array, square circle array, circle square array, five-element square array, plus array and five-element plus square array. The design results of all these seven designs are presented in Section 3 and the design results of sensitivity are also compared.

The metasurface array elements are varied in different shapes to check its effect on the results. The different metasurface array used for the biosensor design is presented in Fig. 2. Total of seven different metasurface elements design is taken into consideration and its results are presented in results and discussions section. The plus shape metasurface array is presented to achieve wideband absorption response [34]. We have used plus shape metasurface array to achieve biomolecule sensing. The electromagnetic behaviour and physical phenomenon metasurfaces and how it helps in improving the sensing structure is studied from [35].

![Fig. 1 Metasurface array-based biosensor design. (a) 3D view of the design (b) 2d top view of the design (c) 2D front view of the design. Circular disks are used as metasurface elements with diameter (Gd) 500nm. The gold array metasurface element thickness is 0.3 μm. The total structure area is 2.5×2.5 μm². The thickness of SiO₂ substrate is 0.5 μm. The graphene monolayer thickness of 0.34 nm. The hemoglobin biomolecules layer thickness is 0.6 μm.](image)
impedance \(z\) we can achieve the permittivity and permeability values of metasurface design using equation (4-5).

\[
\varepsilon = \frac{n}{z} \quad (4)
\]
\[
\mu = n z \quad (5)
\]

Sensitivity analysis:
The sensitivity \(S\) of biosensor is very important parameter and it can be obtained by observing change in wavelength, change in refractive index \(\Delta n\). The equation (6) shows the sensitivity [37]:

\[
S = \frac{\Delta \lambda}{\Delta n} \quad (6)
\]

Graphene conductivity analysis:
Graphene has excellent electrical and optical properties which can be utilized in designing biosensors. The conductivity of graphene monolayer is given by Kubo formula in equations (7-10) and detailed analysis can be found from [38-39]. The permittivity of graphene surface can be calculated from conductivity \(\sigma_s\) and frequency using equation (7).

\[
\varepsilon(\omega) = 1 + \frac{\sigma_s}{\varepsilon_0 \omega \Delta} \quad (7)
\]

Here \(\varepsilon_0\) is vacuum permittivity, \(\omega\)-angular frequency and thickness of graphene monolayer- \(\Delta\) is (0.34nm).

The conductivity is divided into two parts \(\sigma_{\text{intra}}\) and \(\sigma_{\text{inter}}\) and relation between the conductivity and graphene chemical potential is given by equation (8-10).

\[
\sigma_{\text{intra}} = \frac{-j e^2 k_B T}{\pi \hbar^2 (\omega - j 2\Gamma)} \left( \frac{\mu_c}{k_B T} + 2 \ln \left( e^{\frac{\mu_c}{k_B T}} + 1 \right) \right) \quad (8)
\]

\[
\sigma_{\text{inter}} = \frac{-j e^2}{4\pi \hbar} \ln \left( \frac{2|\mu_c| - (\omega - j 2\Gamma) \hbar}{2|\mu_c| + (\omega - j 2\Gamma) \hbar} \right) \quad (9)
\]

\[
\sigma_s = \sigma_{\text{inter}} + \sigma_{\text{intra}} \quad (10)
\]

Here, \(\sigma_{\text{intra}}\)-intra band conductivity, \(\sigma_{\text{inter}}\)-inter band conductivity, \(k_B\) Boltzmann’s constant, \(\hbar\) - Reduced plank’s constant, \(T\) - the room temperature at (300 K), \(\mu_c\) - chemical potential and \(\Gamma\) -scattering rate. Graphene chemical potential is given by \(\mu_c = \hbar v_F \sqrt{\pi C V_{DC}}/e\), \(V_{DC}\) is a gate voltage, \(V_f\) fermi velocity, \(C\)-capacitance and \(\varepsilon_{\text{dl}}\) is dielectric layer static permittivity.

Absorption and reflectance analysis:
The absorption and reflectance of metasurface array-based biosensors can be calculated using the following equations (11-17) and detailed analysis is given in [23]. The reflectance for different incident angle \(\theta_i\) and for the frequency \(\omega\):

\[
r(\omega, \theta_i) = \frac{\omega \cos \theta_i \Pi_{\mu\nu}(\omega, \theta_i)}{2 \hbar c k \omega \cos \theta_i \Pi_{\mu\nu}(\omega, \theta_i)} \quad (11)
\]

\[
\Pi_{\mu\nu}(\omega, \theta_i) \text{ is graphene polarization tensor with } \mu, \nu = 0, 1, 2 \text{ and } \Pi_{\mu\nu} = \Pi_{\nu\mu} \text{. The parallel component of conductivity } \sigma_{\parallel}\text{ can be calculated using equation (12) using graphene polarization tensor. The tangential component of conductivity } \sigma_{\perp}\text{ is not considered as surface conductivity model is considered.}
\]

\[
\sigma_{\parallel}((\omega, k)) = -i \frac{\omega}{4 \pi \hbar k \omega} \Pi_{00}(\omega, k) \quad (12)
\]

Here, \(k\) is the wave vector and the reflectance can be calculated using these conductivity values using equation (13-15).

\[
r(\omega, \theta_i) = \frac{2 \pi \cos \theta_i \sigma(\omega, k)}{c + 2 \pi \cos \theta_i \sigma(\omega, k)} \quad (13)
\]

\[
\mathcal{R}(\omega, \theta_i) = \left| r(\omega, \theta_i) \right|^2 \quad (14)
\]

\[
\mathcal{R}(\omega, \theta_i) = \frac{4 \pi^2 \cos^2 \theta_i \left[ \sigma^2(\omega, k) + 4 \pi^2 \sin^2 \theta_i \right]}{[c + 2 \pi \cos \theta_i \sigma(\omega, k)]^2 + 4 \pi^2 \cos^2 \theta_i \sin^2 \theta_i \sigma(\omega, k)} \quad (15)
\]

For \(\theta_i = k = 0\),

\[
\mathcal{R}(\omega) = \mathcal{R}(\omega, 0) = \frac{4 \pi^2 [\sigma^2(\omega) + 4 \pi^2 \sin^2 \theta_i]}{[c + 2 \pi \cos \theta_i \sigma(\omega)]^2 + 4 \pi^2 \sin^2 \theta_i \sigma(\omega)} \quad (16)
\]

\[
\Lambda(\omega) = 1 - \mathcal{R}(\omega) = T(\omega) \quad (17)
\]

Absorption can be obtained by putting reflectance and transmittance value in the equation (17). When transmittance is very less and near to zero than the absorption can be obtained by using equation (18).

\[
\Lambda(\omega) = 1 - \mathcal{R}(\omega) \quad (18)
\]
 III. RESULT ANALYSIS

The results of the biosensor designs presented in Fig. (1-2) are analyzed using COMSOL Multiphysics and presented in this section. All seven metasurface array biosensor designs are simulated and its results for absorption are presented. The optimized design is obtained from these results.

Optimization of metasurface array biosensor design:

All seven metasurface array biosensor designs (Fig. 2) are simulated under the same conditions to observe its absorption response for the same wavelength range. The results are presented in Fig. 3 for 0.4µm to 0.55µm wavelength range. Absorption response is presented for circle array design (Fig. 3(a)), square array design (Fig. 3(b)), square circle array design (Fig. 3(c)), circle square array design (Fig. 3(d)), five-element square array design (Fig. 3(e)), plus array design (Fig. 3(f)), five-element plus square array design (Fig. 3(g)).

The absorption values are observed for four hemoglobin concentration values. The four different concentrations and their refractive index values are experimentally verified and presented in Table 1.

Table 1. Hemoglobin refractive index values for different concentrations.

<table>
<thead>
<tr>
<th>Concentration (g/l)</th>
<th>Refractive Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1.34</td>
</tr>
<tr>
<td>20</td>
<td>1.36</td>
</tr>
<tr>
<td>30</td>
<td>1.39</td>
</tr>
<tr>
<td>40</td>
<td>1.43</td>
</tr>
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</table>

The wavelength difference of 10nm is observed for two hemoglobin concentrations 10g/l (n=1.34) and 20g/l (n=1.36) for circle array metasurface design presented in Fig. 3(a). The sensitivity obtained using equation (6) is 500nm/RIU. The sensitivity for other designs is also obtained from their absorption response which is presented in Table 2. As presented in Table 2, the highest sensitivity of 500nm/RIU is obtained for circle array metasurface design so the optimized design obtained from this comparison is circle array metasurface design.

Table 2. Comparison of wavelength shift (Δλ) and sensitivity for different designs.

<table>
<thead>
<tr>
<th>Array design</th>
<th>S (nm/RIU)</th>
</tr>
</thead>
<tbody>
<tr>
<td>λ (µm)</td>
<td>Δλ (nm)</td>
</tr>
<tr>
<td>Five-element square array design</td>
<td>450</td>
</tr>
<tr>
<td>Plus array design</td>
<td>250</td>
</tr>
<tr>
<td>Five-element plus square array design</td>
<td>400</td>
</tr>
</tbody>
</table>

Optimized design (Circular array metasurface design) analysis:

We present the metasurface analysis of the optimized design in Fig. (4-6). We have analyzed the optimized design for variation in metasurface thickness and SiO₂ substrate thickness to observe its effect on absorption in Fig. (7-8). The design results in the form of absorption are also compared with air design (n=1) and presented in Fig. (9) The electric field and magnetic field results are also obtained for the optimized design and presented in Fig. 10.

Metasurface analysis:

The permittivity (ε), permeability (μ) and refractive index(n) for the circle metasurface array elements are analyzed for 0.4µm to 0.55µm wavelength range in Fig. (4-6) respectively. This wavelength range is selected because of the highest peak of absorption is available in this range. The real and imaginary parts represented in the results. The results of the permittivity, permeability, and refractive index are calculated by putting the values of reflection and transmission results in equations (1-5). The permittivity results presented in Fig. 4 show the negative values of real part of the permittivity at three wavelengths around 0.41µm, 0.45µm, and 0.51µm. The real part of permittivity is showing these negative peaks which clearly show the metasurface effect.

The permeability values of the circle array metasurface design are presented in Fig. 5. The real values of the permeability are clearly showing the negative behavior same as that of permittivity values but the difference in values is visible. The refractive index values also following the same behavior and its results are presented in Fig. 6.

We have simulated the optimized design (circle array metasurface biosensor design) for variation in metasurface thickness (Fig. 7) and SiO₂ substrate thickness (Fig. 8) to observe its effect on absorption. The metasurface gold layer thickness is changed from 0.1µm to 0.6µm in Fig. 7. The electric field and magnetic field results for variation in metasurface thickness and SiO₂ substrate thickness (Fig. 8) to observe its effect on absorption in Fig. (7-8). The absorption values are observed for four hemoglobin concentration values. The four different concentrations and their refractive index values are experimentally verified and presented in Table 1.

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The wavelength difference of 10nm is observed for two hemoglobin concentrations 10g/l (n=1.34) and 20g/l (n=1.36) for circle array metasurface design presented in Fig. 3(a). The sensitivity obtained using equation (6) is 500nm/RIU. The sensitivity for other designs is also obtained from their absorption response which is presented in Table 2. As presented in Table 2, the highest sensitivity of 500nm/RIU is obtained for circle array metasurface design so the optimized design obtained from this comparison is circle array metasurface design.
The SiO$_2$ substrate thickness is varied 0.3 µm to 0.8 µm to observe its effect on the absorption performance of biosensor.

Fig. 3 Absorption response of different metasurface array-based biosensor designs (a) circle array (b) square array (c) square circle array (d) circle square array (e) five-element square array (f) plus array (g) five-element plus square array. The wavelength difference of 10nm for refractive indexes of 1.34 and 1.36 gives the highest sensitivity of 500nm/RIU.
We have also simulated the circle array design for different circle radius ranging from 0.2 µm to 0.4 µm. From the results of Fig. (7-9), it is clear that the absorption is more than 50% and increasing with wavelength for 0.45 µm and 1 µm wavelength range and optimized values of circle gold metasurface layer thickness is 0.3 µm, SiO₂ layer thickness is 0.5 µm and circle gold metasurface radius is 0.25 µm.

The comparative plot of metasurface array biosensor design with hemoglobin as biomolecules and air are presented in Fig. 10. From the figure, it is observed that the peak wavelength difference is observed at 120 nm. The refractive index difference is 0.34 and the sensitivity for this design comes up to 353 nm/RIU. The electric field and magnetic field response are presented in Fig. 11 for four different wavelengths for circle array metasurface design. The four different wavelengths are considered to show electric and magnetic field concentration which proves the resonance effect. The electric field and magnetic field response are better for 0.455 µm wavelengths compared to other wavelengths which show that absorption is higher for this 0.455 µm wavelength compared to other wavelengths.

The comparative analysis of the proposed biosensor design with previously published different designs [14. 29-31] is presented in Table 3. From the comparison, it is clear that our proposed design is better compared to other absorber biosensor designs.
The circle array design physical geometrical parameters presented. The optimized circle array biosensor design (n=1.34). The wavelength range observed is 0.1 μm to 1 μm. The wavelength peak is having a difference of 12 nm.

![Image](image.png)

**Fig. 11 Electric and magnetic field for (a) 0.3 μm (b) 0.455 μm (c) 0.76 μm (d) 0.90 μm**

**Table 3.** The comparison of the sensitivity of the proposed design compared to the previously published designs [40, 41].

<table>
<thead>
<tr>
<th>Design</th>
<th>Sensitivity (nm/RU)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hemoglobin refractive index sensor from Reference [40]</td>
<td>387</td>
</tr>
<tr>
<td>Hemoglobin refractive optical biosensor from Reference [41]</td>
<td>322</td>
</tr>
<tr>
<td>Proposed circle array metasurface biosensor (hemoglobin concentrations)</td>
<td>500</td>
</tr>
<tr>
<td>Proposed circle array metasurface biosensor (hemoglobin-air)</td>
<td>353</td>
</tr>
</tbody>
</table>

The main advantage of using circle array biosensor is its easy design which can be easily fabricated. The different biosensor configurations proposed in this paper can be used to sense other biomolecules like urine, etc. The gold material absorbs biomolecules poorly which reduces the sensitivity but sensitivity can be improved further by using alternate material which can absorb more biomolecules than gold material. The fabrication of metasurface array designs proposed can also be easily fabricated as presented in [42]. The gold metasurface array is placed above SiO₂ separated by graphene monolayer sheet. The procedure of testing is comprised as light incidence on the surface of structure, absorption of bio molecules and detection by spectrum analyzer.

**IV. CONCLUSION**

Sensitivity is a very important parameter of any biosensor. We have presented a sensitivity analysis of seven different gold metasurface array designs. The sensitivity of these seven designs (circle array, square array, square circle array, circle square array, five-element square array, plus array and five-element plus square array) are compared. From the comparison, circle array metasurface design gives the highest sensitivity of 500 nm. The absorption analysis for four different concentrations of hemoglobin biomolecules is presented. The circle array design physical geometrical parameters are optimized. The optimized values of 0.3 μm for gold circle metasurface thickness, and 0.5 μm for SiO₂ substrate thickness, and 0.25 μm for gold circle metasurface radius are obtained. The optimized circle array biosensor design is compared with previously published designs [14, 40-41]. The optimized circle array biosensor can be used in biosensing medical applications.

**Acknowledgments**

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