Design of novel sensitive terahertz metamaterial absorbers based on graphene-plasmonic nanostructures

Atefeh Chahkoutahi1 · Farzin Emami2

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Abstract
In this paper, four different configurations of sensitive metamaterial absorbers based on graphene-plasmonic combinations are designed and proposed. The nanostructures are made of graphene, SiO2, aluminum and gold layers on a silicon substrate. Graphene-ring shaped structures with diagonal strips in vertical and horizontal directions are considered in the structures which greatly affect the absorption characteristics (absorption peak value and wavelength). Aluminum layer is used in the structure to prevent the transmission of light throughout some layers and improve the absorption factor. To promote the functionality of the structures, effects of the structural parameters ($R_1$ and $R_2$) and chemical potentials ($E_{f1}$, $E_{f2}$, $E_{f3}$ and $E_{f4}$) on the absorption peak are also studied. The four individual configurations with different layers and strip directions demonstrate distinct and different wavelength ranges; structure-1: 45–60 µm, structure-2: 50–70 µm, structure-3: 70–85 µm, and structure-4: 80–100 µm. Thus, they can be utilized for wide categories of applications. Sensitivities of 1500 nm/RIU, 2250/RIU, 3750 nm/RIU and 4850 nm/RIU are obtained for four types, respectively. The proposed structures can be categorized as refractive index biosensors, which indicate acceptable sensitivities and can be used for detection of different elements like hemoglobin and glucose in blood samples.

Keywords Biosensor · Graphene · Nanostructure · Plasmonic · Refractive index sensor

1 Introduction
In a recent decade, photonic biosensors have achieved specific and popular attentions by researchers. Different optical methods are proposed for bio-sensing structures, in which surface plasmon resonance (SPR) is supposed to be the preferable one due to its efficient
functionalities, flexible designing, compact size, remote sensing and other important characteristics (Panda 2020).

Indeed, SPR-refractive index (SPR-RI) biosensors have attracted extreme attentions (Rahman 2020). Biosensors can be utilized as diagnosis instruments, clinical and lab detection devices (Ouyang et al. 2016; Hossain and Rana 2016), and also for sensing various bio-molecules such as proteins (Tian 2019), DNA (Wang 2020) and other vital tissues. SPR based sensors have interesting and appropriate specifications that make them good candidates for bio-sensing applications. Actually SPR refers to the interaction of oscillatory electrons and electromagnetic (EM) waves at the interface of metal and dielectric layers, which causes the confinement and increment of the optical fields at sub-wavelength dimensions (Rafiee et al. 2019a). Graphene-plasmonic nanostructures can be scaled down to nano-meter dimensions as they can conquer the diffraction limits of light (Rafiee et al. 2019b). Terahertz (THz) radiations with frequencies between 0.1 THz to 10 THz have also gained great interests (Hajati 2020). THz technology spans the operating regions from millimeter to infrared spectrum which covers many different applications. Graphene-plasmonic devices indicate better sub-wavelength confinements, lower losses, and EM tunability and thus are appropriate for operating in THz spectrum (Hajati 2020; Jablan et al. 2009).

Different kinds of SPR-based biosensors had been proposed based on various dielectric media, metal types and different layers of graphene. Recently, an SPR biosensor was suggested for sensing glucose concentration in blood and gas with different RIs (Panda 2020). This biosensor indicated acceptable sensitivities of 275.15˚/RIU and 92.1˚/RIU for glucose and gaseous analyte.

In another research, an infrared biosensor for nano-fluidic analysis based on graphene plasmonics, which detected the change of RI by the wavelength shift of resonant dips, was reported (Wei et al. 2014). The sensitivity amount of 1920 nm/RIU was obtained for this biosensor. A graphene based biosensor for obtaining plasmonic induced transparency (PIT) with appropriate functionalities in mid-IR region, was suggested (Vafapour 2017). Biosensors for detecting vibrational fingerprints could be realized for bio-analytical and pharmaceutical applications by using periodic graphene nano-ribbons (Cai 2019). A graphene plasmonic biosensor for detection of colorless biomaterial was proposed and developed with sensitivity of 333.3 nm/RIU and figure of merit (FOM) of 16.665 RIU (Farmani 2020). Also, in another work (Sharma et al. 2018), a chalcogenide fiber optic sensor with graphene layer was proposed for detection of hemoglobin in human blood. All in all, nowadays graphene-based biosensors are of great interest to scientists and researchers. As a result, four different structures based on graphene-plasmonic combinations are proposed for bio-sensing applications.

2 Structure description and theory

Consider a simple structure as shown in Fig. 1, which is consisted of a graphene pattern on the top, a silicon dioxide layer ($\text{SiO}_2$), an aluminum (Al) layer and a silicon ($\text{Si}$) substrate. Figure 1 is the side view of Fig. 2a.

The relation between the transmission, absorption and reflection fields can be considered based on the simple relation of Chen (2019), Li (2019):

$$A(\omega) = 1 - R(\omega) - T(\omega)$$

(1)

in which, $R(\omega) = |S_{11}(\omega)|^2$, $T(\omega) = |S_{21}(\omega)|^2$, where the scattering parameters $S_{11}(\omega)$ and $S_{21}(\omega)$ are the reflection and transmission coefficients.
The Al-layer is used in order to prevent the passage of the incident light through the first two layers (Li 2019). For blocking the transmission of the incident light, the thickness of Al is chosen to be greater than the penetration depth of light in the IR-region (Li 2019). Therefore $T(\omega) = |S_{21}(\omega)|^2 = 0$ and $A(\omega) = 1 - R(\omega)$ are considered.

To achieve the perfect absorber (for sensing applications), the reflection parameter $R(\omega)$ must be equal to zero so that, $A(\omega)$ becomes 1 and hence the incident light would be completely absorbed. In order to have the acceptable absorption, optimized parameters should be considered for the structure. As depicted in Fig. 1 c, the absorption peak values of 98 and 99.1 occur at 41 µm and 54 µm, respectively.

Special optical properties of graphene can lead to the production of great opacity in vacuum with absorption of about 2.3% of light. The light absorption can be increased for different designs of graphene and surrounding layers. The surface conductivity of a graphene layer can be calculated from the Kubo formula which is a function of different parameters such as wavelength, temperature and chemical potential (G.W., Hanson 2008):

$$\sigma_g(\omega, E_f, \Gamma, T) = \sigma_{g\text{--real}} + j\sigma_{g\text{--imag}} = \sigma_{\text{intral}} + \sigma_{\text{inter}}$$  \hspace{1cm} (2)

where $\omega$, $E_f$, $\Gamma$ and $T$ indicate the operation frequency, the chemical potential, the phenomenologial scattering rate ($\Gamma \equiv 1/2\tau$, $\Gamma$ is the scattering time) and the absolute temperature, respectively.

The intra-band and inter-band electro-photon scattering parameters can be described as (Hanson 2008):
where \( k_B \) and \( e \) are the Boltzmann constant and the electron charge.

The dielectric function of the metals can also be described by the Drude model (Hanson 2008; Emami 2018, 2019):

\[
\varepsilon(\omega) = \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 - j\omega\gamma} \quad \text{(5)}
\]

where \( \varepsilon_\infty = 3.7 \) (dielectric constant at infinite frequency), \( \gamma = 0.018 \) eV (collision plasma angular frequency) and \( \omega_p = 9.1 \) eV (bulk plasma angular frequency) (Hanson 2008; Emami 2018, 2019).

In the following section, different configurations with their results are presented.
3 Results and discussions

In this Sect. 4 different structures (models) based on of graphene-plasmonic nanostructures and their functionalities as biosensors are considered. It is important to note that the strips situated in the middle of the rings can greatly affect the characteristics of the structures. They can steer the direction of light to improve field distributions at specific wavelengths (Li 2019). Therefore, their effects on the absorption spectrum will be discussed.

3.1 First structure

The first proposed structure with its side view (unit cell) is presented in Fig. 2. The figure indicates the absorption, transmission and reflection spectrum.

As shown in this figure, it is consisted of a periodic graphene pattern. The geometrical parameters of Fig. 2 are tabulated in Table. 1.

Simulation results reported in Fig. 0.2c, was obtained by the finite difference time domain (FDTD) method. Field distribution for this structure in different wavelengths can be seen in Fig. 3.

To improve the functionality of the proposed structure, effects of different geometrical parameters such as $R_1$ (ring width), $R_2$ (strip width, refer to Fig. 2 b), chemical potential ($E_f$) on the wavelength and value of the absorption spectrum are investigated. Figure 4 shows simulation results for different values of $R_1$ and $R_2$, while other parameters are kept constant.

As can be seen from Fig. 4a, by considering $R_1=0.1 \, \mu m$, increasing $R_2$ would lead to the blue shift of the absorption peak-wavelength and would decrease the absorption peak. The best result is obtained for $R_2=0.1 \, \mu m$ with the absorption peak of 99.7%. In Fig. 4b, by considering $R_2=0.1 \, \mu m$ and $R_1=0.1 \, \mu m$, the absorption peak wavelength would experience the blue shift with the absorption peak of 99.9%. As a result, for obtaining the perfect absorber with nearly perfect absorption peaks, $R_1$ and $R_2$ should equal to 0.1 $\mu m$. The variations of $R_1$ and $R_2$ can be explained by a simple LC resonant circuit. In the LC circuit, the upper and lower parts of the graphene make the two capacitors and the surface current is excited between the graphene and Al layers which would limit the incident light and lead to the perfect absorption (Li 2019; Zhang et al. 2006).

Another important parameter is the chemical potential, $E_f$. Effects of various chemical potentials on the absorption spectrum are reported in Fig. 5.

| Table 1 | Parameter values for Fig. 2 |
|---------|-----------------------------|
| Parameter | Value ($\mu m$) |
| $R_1$ | 0.1 |
| $R_2$ | 0.1 |
| $D$ | 1 |
| $h_1$ | 5 |
| $h_2$ | 4.7 |
| $W$ | 2.4 |
| $A$ | 0.5 |
| $B$ | 2.4 |
Fig. 3 Field distribution for the first proposed structure, $E_{f1}=0.7$ eV and a $\lambda = 50 \ \mu m$, b $\lambda = 52 \ \mu m$, c $\lambda = 54 \ \mu m$, d $\lambda = 56 \ \mu m$

Fig. 4 Absorption spectrum of the first proposed structure for: a $R_1=0.1 \ \mu m$ with different values of $R_2$, b $R_2=0.1 \ \mu m$ with different values of $R_1$

Fig. 5 Schematic of the absorption spectrum versus wavelength for different values of $E_{f1}$
As can be seen from this figure, the absorption peak wavelength would have a blue shift, as $E_f$ is increased. Again, this phenomenon can be explained by the circuit theory. In this theory, graphene can be described as a shunt admittance which can be varied by the geometrical parameters ($R_1$, $R_2$) and chemical potential ($E_f$) (Xu 2018; Arik 2017). Therefore, changing $E_f$ can alter the absorption peak wavelength according to the following equation (Li 2019; Zhang 2018):

$$
\lambda = 2\pi \frac{c}{\sqrt{LC}}
$$

(6)

where $c$, $L$ and $C$ are speed of the light in vacuum, capacitance and inductance, respectively. Enhancing $E_f$ would diminish the inductance value $L$ (Liu 2018), which would decrease the absorption peak wavelength according to (6). Considering $E_f=0.9$ eV, the short wavelength ranges of 30–5 µm with 97% absorption peak and long wavelength ranges of 45–60 µm with 94% peak, would be achieved. So, in the following parts $E_f=0.9$ eV is selected.

The proposed structure of Fig. 2 can be used as a biosensor with acceptable sensitivity. The absorption spectrum for materials with different refractive indices (2.32, 2.38, 2.44 and 2.5) can be seen in Fig. 6.

As indicated in figure, increasing RI would increase the absorption peak wavelength (Hajati 2020; Chen 2018) and the sensitivity factor $[\Delta \lambda / \Delta n]$ of 1500 nm/RIU can be obtained.

### 3.2 Second structure

By considering 4 gold triangles at the corners and one square in the center of Fig. 2, second proposed arrangement of the biosensor would be presented. This shape is depicted in Fig. 7.

The field distribution in the second structure at different wavelengths (resonant and non-resonant wavelengths) can be seen in Fig. 8.

As can be seen, the strips affect the field distribution for different wavelengths.

Effects of chemical potential ($E_f$) variations on the absorption spectrum are studied and the simulation results are plotted in Fig. 9.

As stated for $E_f$, by increasing $E_f$ from 0.55 eV to 0.8 eV, the absorption peak wavelength would be blue shifted, which can be described by the circuit theory. Considering $E_f=0.8$ eV, the short wavelength ranges of 38–50 µm with 96% absorption peak and long wavelength ranges of 50–70 µm with 98.5% peak are achieved. For the following simulations, $E_f=0.8$ eV is selected.
By considering the second structure as the biosensor, the absorption spectrum for materials with different refractive indices (2.059, 2.106, 2.153 and 2.2) can be depicted in Fig. 10.

From Fig. 10, it can be seen that, increasing RI would shift the absorption peak wavelength to higher values (materials with higher refractive indices can confine the light...
waves stronger than lower ones) (Hajati 2020; Chen 2018). For the second structure, the sensitivity value of 2250 nm/RIU can be achieved.

### 3.3 Third structure

In the third proposal, by adding half circles of gold to the second structure, another configuration of the biosensor would be presented. This third suggested structure, with half circles of gold blocks, is depicted in Fig. 11. The parameters $F = 0.35 \, \mu m$, $h_3 = 0.5 \, \mu m$ and $e = 0.35 \, \mu m$ are considered for this configuration.

Field distribution in the third structure at different wavelengths (resonant and non-resonant wavelengths) can be shown in Fig. 12.

For better understanding of the functionality of the third structure, effects of chemical potential ($E_{f3}$) on the absorption spectrum were studied. Simulation results are shown in Fig. 13.

As can be seen in Fig. 13, by enhancing $E_{f3}$ from 0.4 eV to 1.2 eV, the absorption peak wavelength would be blue shifted, and it may also be explained by the circuit theory (Li 2019; Zhang 2018). Considering $E_{f3} = 1 \, eV$, the short wavelength ranges of 60-75 $\mu m$ with 97% absorption peak and long wavelength ranges of 70-85 $\mu m$ with 99% peak are achieved. For the following simulations, $E_{f3} = 1 \, eV$ is used.

To consider the third structure as the biosensor, the absorption spectrum for materials with different refractive indices (1.335, 1.357, 1.379 and 1.405) are shown in Fig. 14 (these refractive indices are related to different hemoglobin concentrations) (Sharma et al. 2018).

The variation of absorption peak wavelength for the third proposal is the same as the first and second structures; increasing RI shift the wavelength to higher values (Hajati
Fig. 11  a Schematic of the third proposed structure, b side view of the proposed structure

Fig. 12  Field distribution in the third proposed structure for $E_{f3} = 0.9$ eV at: a $\lambda = 70$ µm, b $\lambda = 71$ µm, c $\lambda = 72$ µm, d $\lambda = 73$ µm
For the present case, the sensitivity value of 3750 nm/RIU can be achieved.

### 3.4 Fourth structure

In this section, by changing the strip direction of third structure (two vertical directed strips instead of horizontal stripes), another configuration of the biosensor would be presented.
which contains one absorption peak in the wavelength range of 80–100 µm. The suggested structure is shown in Fig. 15.

The field distribution of the fourth structure at different wavelengths (resonant and non-resonant wavelengths) can be depicted in Fig. 16.

For studying the characteristics of this case, effects of its chemical potential ($E_{f4}$) on the absorption spectrum are also considered. Simulation results are shown in Fig. 17.

As can be seen, by enhancing $E_{f4}$ from 0.6 eV to 1.2 eV, the absorption peak wavelength would have a blue shift (like the three other structures) (Sharma et al. 2018). Considering
$E_{f4} = 0.9 \text{ eV}$, the wavelength ranges of 80–100 µm with 99.9% absorption peak is achieved. For the following simulations, $E_{f4} = 0.9 \text{ eV}$ would be considered.

To consider this structure as the biosensor, the absorption spectrum for materials with different refractive indices (1.375, 1.365, 1.352 and 1.338) are plotted in Fig. 18 (these refractive indices are related to different glucose concentrations in blood samples; $n = 1.375$ for 100 mg/dl, $n = 1.365$ for 75 mg/dl, $n = 1.352$ for 50 mg/dl, $n = 1.338$ for 25 mg/dl) (Panda 2020).

It can be seen from Fig. 18, that enhancing RI has led to the increment of the absorption peak wavelength (as increasing the refractive index would lead to higher confinement of the light-wave) (Hajati 2020; Chen 2018). For this case, the sensitivity value of 4850 nm/RIU can be obtained.

### 4 Conclusion

Four different structures based on graphene-plasmonic nanostructures were proposed for bio-sensing applications. The proposed systems were consisted of graphene, $SiO_2$, Al and gold layers on the silicon background. Combinations of ring-shaped graphene layers with different strip directions resulted in various absorption specifications (affect the absorption peak value and wavelength). For conducting better investigation on the characteristics of the proposed structures, effects of geometrical and chemical potential on the absorption spectrum were also considered. The first, second, third and fourth suggested structures indicated sensing functionalities at 45–60, 50–70, 70–85 and 80–100 µm ranges, with the sensitivity factors of 1500 nm/RIU, 2250/RIU, 3750 nm/RIU and 4850 nm/RIU, respectively. As a result, by introducing the four proposed structures, tunable biosensors appropriate for various applications like sensing different hemoglobin and glucose concentrations in blood samples were obtained.

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