Numerical analysis on DNA-sensor based on copper-graphene surface plasmon resonance

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***Abstract*—This paper numerically presents a highly sensitive surface plasmon resonance (SPR) graphene-based biosensor by taking high adsorption efficiency of graphene into consideration. The pi-stacking interaction between carbon-based hexagonal structure of graphene with carbon-based ring biomolecules such as single-stranded DNA is the key factor behind this efficiency. Graphene layers added to a conventional copper SPR biosensor causes a drastic sensitivity enhancement. In comparison to conventional SPR sensors this produces a larger change in the refractive index at the metal-dielectric interface. The light reflection coupled into a SPR mode propagating along a copper-graphene layer is calculated and compared to a conventional SPR sensor. The proposed SPR sensor could then not only be applied for highly sensitive but also for cheap DNA-biosensor.**

Keywords— surface plasmon resonance, biosensor, graphene, copper.

I. Introduction

Nowadays DNA sensors have an important role in diagnostic tests for early stage of cancer detection, gene sequence Analysis, forensic science, and health assessment. Consequently, a wide variety of DNA biosensors based on different detection techniques has been studied [1, 2]. Among these techniques, electrochemical DNA biosensors are particularly attractive because of their simplicity, low cost, high sensitivity and miniaturization. To date, various electrochemical DNA biosensors have been reported. In recent years, there are lots of significant researches in the field of plasmonics. The properties of many nanoscale metallic structures have been extensively explored for use as surface plasmon resonance DNA-sensor.

Surface plasmons (SPs) are waves that propagate along the surface of a noble metals such as gold, copper and silver in visible range. The SP waves at a metal-dielectric interface is applicable as kind of robust and label-free electrochemical biosensor which called surface plasmon resonance (SPR) biosensor. The SPR biosensor shown as a very effective optical detection for absorption of biomolecules [3, 4].

This is due to the great change in the excitation angle of SP which made by variation in the refractive index on the binding layer on top of the metal layer. In addition to the simplicity of this configuration, it is an extremely sensitive to variations of refractive index near the metal surface.

In a conventional SPR sensor, a thin metal layer is sandwiched between two dielectrics, as shown in Fig. 1.

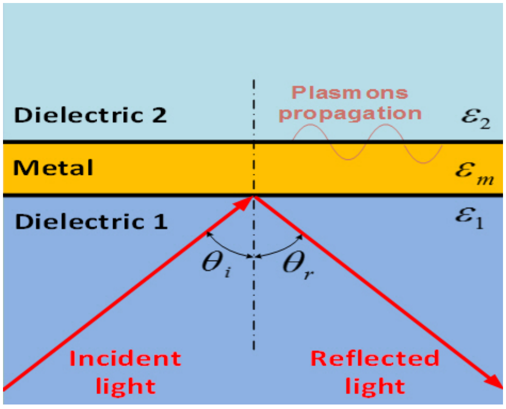

Fig. 1. Excitation of surface plasmon in dielectric-metal-dielectric structure.

SPR sensors can be classified by coupling wavelength, coupling angle, and intensity, phase, or polarization changes [5]. Gold and silver are weak biomolecule absorbers, restricting the sensitivity of the sensor. Oxidation of the metal surface can further restrict sensitivity. The surface plasmons properties can be tailored by functionalizing of metal surface.

Several strategies have been suggested for improving sensitivity such as metallic nanoslits, metal nanoholes and nanoparticles in buffered solution. The accurate control of the optical properties and geometry of nanostructure still remains challenging though. Functionalization with biomolecular recognition elements (BRE) is an alternative for improving the biomolecule adsorption at the metal layer. The combination of graphene as a BRE with plasmonics could result in fast, relatively cheap and small active optical biosensor.

II. Graphene Optical Properties

Graphene could play a significant role in new generation of multilayer optical devices consisting of almost all kinds of optical materials such as dielectrics, semiconductors, semimetals, metals [6]. It can be used as a gapless material or the one have small and large optical gaps. A mixture of graphene with conventional plasmonic nanodevices may offer ultrasensitive chemical sensors and biosensors. It expects that graphene has a very high quantum effectiveness for light–matter interactions. Furthermore, its optical and electrical properties can be altered by doping and gating in conventional plasmonics devices based on noble metals.

Recent studies on transmission of light through graphene membranes revealed a universal opacity constant of graphene (wavelength independent) [7]. By using the Fresnel coefficients calculation framework the refractive index in the visible spectrum is obtained from [8, 9]:

$$n_{Graphene} = 3 + i(1.8153\times10^{6})\lambda_0 \tag{1}$$

where λ_0 is the free space wavelength.

The graphene surface is a better absorber of biomolecules, due to the π-stacking interactions between graphene's hexagonal cells and the carbon-based ring structures in biomolecules [10, 11].

III. Design Consideration and Theoretical Model

In this study, a graphene sheet on top of the copper thin film is considered as a BRE. In recent years, graphene on Au has been fabricated and shows stable adsorption of biomolecule with carbon-based ring structures [12]. In comparison with a conventional SPR sensor, graphene provides a greater change of refractive index near the metal surface. In addition a grapheme coating on the copper surface improves the surface plasmon polariton (SPP) propagation constant and prevents oxidation.

The set up for proposed biosensor is illustrated in Fig. 2, where the graphene layer covers a copper thin film. The other side of copper layer is in contact with SF10 glass. Considering the intensity of light reflected from a N-layer system for a transverse-magnetic incident wave, the total reflection, R, is given by [13]

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

$$M_{ij} = \left(\prod_{k=2}^{N-1} M_k\right)_{ij}, i, j = 1, 2 \tag{3}$$

$$M_k = \begin{bmatrix} \cos\beta_k & -i\sin\beta_k / q_k \\ -iq_k\sin\beta_k & \cos\beta_k \end{bmatrix} \tag{4}$$

$$q_k = \frac{\sqrt{\varepsilon_k - n_1^2\sin^2\theta}}{\varepsilon_k} \tag{5}$$

$$\beta_k = d_k\left(\frac{2\pi}{\lambda}\right)\sqrt{\varepsilon_k - n_1^2\sin^2\theta} \tag{6}$$

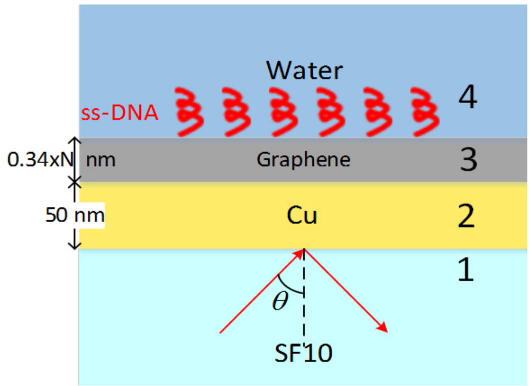

Fig. 2. Schematic of graphene-based SPR biosensor.

The k_{th} layer, where k is from 2 to N-1, has a thickness of d_k and local dielectric function ε_k. The scenario considered uses a 50 nm copper film with multiple layers of graphene (d_3) as the BRE. Thickness of each graphene layer is 0.34 nm. In this study we considered a fixed wavelength of 633 nm which is for He-Ne laser. The calculations were carried out for the dielectric function of copper using a Drude-Lorentz model. Binding layer of DNA hybridization with 3 nm thickness are modeled as a homogeneous layer with an initial refractive index of 1.462 in a water medium and the refractive index of water is 1.33 respectively.

The sensitivity (S) can be defined by relation between the sensor output, θ, angle of incidence light, and the moles of biomolecules in the water, M [14]:

$$S = \frac{\Delta\theta}{\Delta M} = \frac{\Delta\theta}{\Delta n}\times\frac{\Delta n}{\Delta M} = S_n E \tag{7}$$

Where Δn is the change in refractive index at the copper surface.

The enhanced adsorption efficiency of biomolecules by using graphene is given by $E_{Graphene} = A.E_{conventional}$ (where A>1).

IV. Results and Discussion

Fig. 3 shows the numerically simulated SPR curve (red graph) for the conventional biosensor when there is not any biomolecules. A minimum reflection in red curve is due to the excitation of the surface plasmon polariton. The green curve shows the absorption and blue graph indicates the transmission of light, respectively. As shown, the SPR occurred in total internal reflection. There is no transmission of light for all the incident angles bigger than 50 degree.

By adding the DNA on top of the copper surface, refractive index of the region near the copper surface will be changed causing a shift in SPR curve as shown in Fig. 4. It can be seen that the change in the refractive index of the water near to the sensor surface, due to biomolecule adsorption, results in a shift in the angle of the minima.

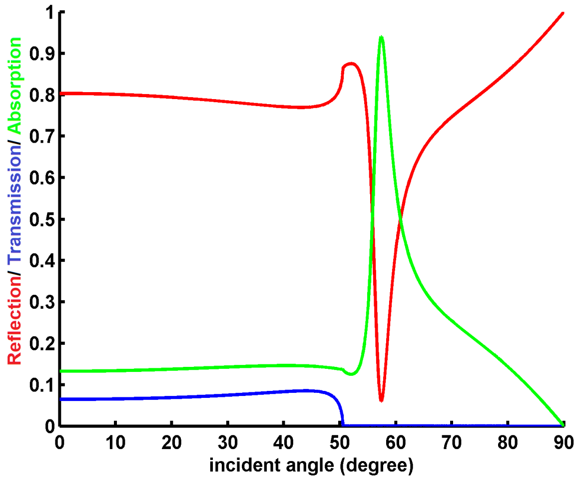

Fig. 3. Reflection, transmission and absorption of light in conventional copper SPR sensor based on Fresnel equation.

The effect of multilayer graphene in SPR curve is calculated, based on transfer matrix for N-layer Fresnel equation, as shown in Fig. 5. It is clearly illustrated that by adding more graphene layers on the top of copper surface, the SPR curve will be broaden, resulting in less sensitivity. Therefore the maximum thickness of the graphene layer to get the suitable output should be noticed. The results summarized in Table 1 shows that the shift increases with an increase in number of graphene layers.

The calculations indicated that the sensitivity to refractive index is enhanced by 6.5% for each layer of graphene derived from table 1. The total sensitivity enhancement can obtained by $W = (1 + 0.065N)A$, where N is the number of graphene layers and A is the coefficient of adsorption efficiency. It has been reported that A could be as high as 4 [14], giving about 5.3 times increase in sensitivity for five layer graphene.

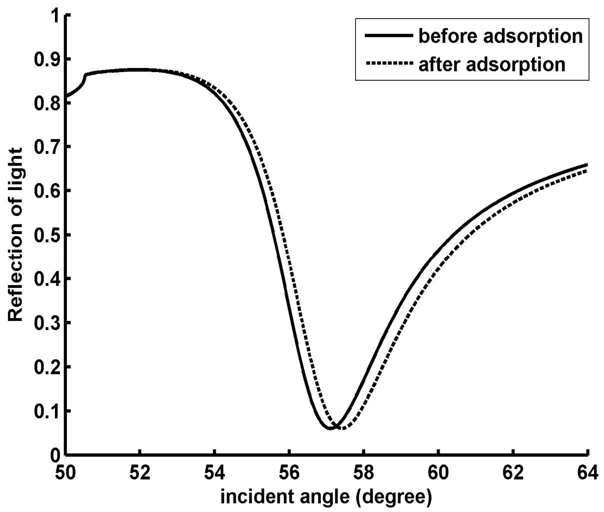

Fig. 4. SPR curve before (solid line) and after (dashed line) adding DNA in conventional structure.

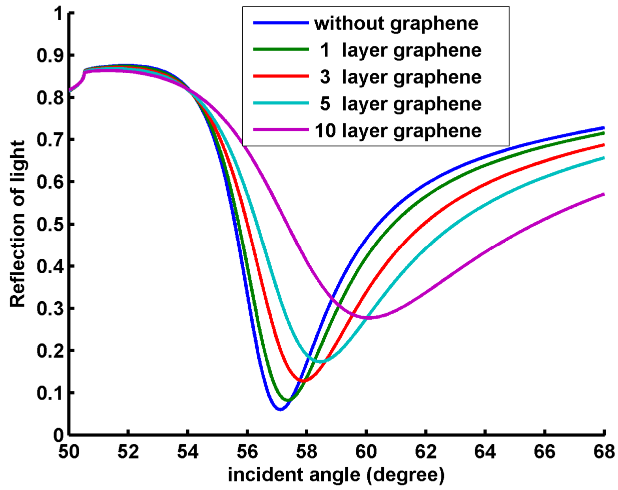

Fig. 5. SPR curves for conventional structure and graphene-based structure.

The incidence angles at minimum point are known as SPR angle such as θ_{SPR1} and θ_{SPR2}. These refer to the angles before and after adsorption of biomolecules on graphene surface. It is shown in table 1 that by adding more graphene layers, the resonance angle shift will be greater due to the larger change in refractive index at sensing medium near to the graphene surface.

Table 1: sensitivity enhancement by using multilayer graphene.

Graphene layer	θ_{SPR1}	θ_{SPR2}	$\Delta\theta$ (degree)	S_n	W
0	57.1	57.41	0.31	2.348	----
1	57.35	57.68	0.33	2.5	4.26
3	57.88	58.25	0.37	2.803	4.78
5	58.47	58.88	0.41	3.106	5.3
10	60.1	60.51	0.51	3.863	6.6

V. CONCLUSION

The sensitivity for a copper-graphene SPR biosensor have been presented by using MATLAB simulation. The results showed that by using a graphene layer on copper surface in a SPR biosensor has an enhanced sensitivity as compared to that of a conventional sensor. This is primarily due to a better adsorption efficiency of graphene and greater change in refractive index near the copper surface. The model suggested that the total sensitivity increases with the number of graphene layers used.

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