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Variable Incidence Angle Subwavelegth Grating SPR Graphene Biosensor

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***Abstract*— This paper investigates the sensitivity enhancement of a variable incidence angle subwavelength grating based multilayer surface plasmon resonance biosensor (SPRB). In the proposed design, a periodic array of subwavelength grating is integrated on top of a layer of graphene sheet in the multilayer SPR biosensor. The performance of the biosensor is investigated through monitoring the biomolecular interactions of cDNA-ssDNA interactions on its surface. The sensitivity improvement is indicated by the shift of the resonance peak angle.**

I. Introduction

SURFACE plasmon resonance is an optical phenomenon whereby an electro-magnetic wave propagating along the surface of a thin metal layer. It is based on the total internal reflection at the metal-dielectric interface. Excitation of surface plasmon (either by light or by electron bombarding) is required to get the resonance oscillation. The excitation of surface plasmon (SP) can be accompanied either by varying incidence angle or by varying the wavelength of the optical laser beam. Thus, the detection of target biomolecule can be made either by measuring the shift of incidence angle or wavelength at resonance. Angle integration in SPRB is the widely used approach because of its low angular resolution. A number of SPRB platforms have been reported including attenuated total internal reflection, optical fiber, optical waveguide, and intensity measurement [1-3] which are capable of sensing target biomolecules on their sensing surfaces.

Enhanced detection sensitivity in SPRB is crucial for low molecular detection which be achieved by means of creating local hot spots as well as increased reaction area generated by the near-field interactions around the nano-sized metallic structures [4, 5]. Improving the sensing area through the proper immobilization of receptor molecule and also preventing the unspecific adsorption will avail to boost the sensitivity [6]. Furthermore, it can also be obtained with many different techniques and geometrical optimization which includes incorporating a graphene sheet on top of gold thin film, periodic nanograting arrays [7-11], phase variation [12], etc. Intensive research has already been directed towards boosting the sensitivity [10, 13]. Among these methods, phase detection and colloidal metallic nanoparticles have been considered extensively [14, 15]. Phase produces more rapid changes compared to intensity which facilitates the faster detection. However, its disadvantages include suffering from a small dynamic range [16]. On the other hand, incorporating colloidal nanoparticle can amplify the SPR signals and hence enhance the sensitivity [8]. However, this method has a certain limitations towards application-specific variations depriving desirable sensitivity characteristics [14].

Whilst most of the existing studies used nanoparticles and phase based detection, we have employed the periodic dielectric nanograting on a graphene layer as an alternative means to excite the SPs for improved field amplification and thus the sensitivity. The sensitivity enhancement is inevitably accompanied by a limited surface increase of reaction area and structural perturbation of the periodic dielectric nanograting on the graphene layer deposited on a thin gold film [6].

II. Detection Principle

In SPR, the strength, decay characteristic and distribution of the field are much affected by the operating wavelength and polarization. The SPR signal is therefore becomes sensitive to changes to any of these parameters. Since the adsorption of target biomolecules on the sensing surface produces a change of RI, a shift of resonance peak in SPR spectrum is measurable. This shift of resonance peak upon the introduction of the target bimolecules gives an indication of detection of the target biomolecule.

In our investigation, the simulation is considered using Kretschmann configuration where a prism is placed against a gold thin film. And, subwavelength nanograting followed by a graphene layer on top of the gold thin film is constructed in this configuration. The outer surface of the grating layer is immobilized with a target biomolecule. Resonance of the SP oscillation occurs and hence a dip in the reflectivity curve is found when any of the SPR conditions (e.g., incidence angle, wavelength) is met. Then, the biomolecular interaction between the captured target and receptor molecules alters the resonance condition which causes to shift the resonance peak.

To monitor the binding event in the proposed biosensor, graphene grating based surface plasmon resonance biosensor (called GG-SPRB), the field profile is investigated before and after the detection of biomolecules. The incidence angle is tuned to setup a resonance condition. As can be seen from Fig. 1, both the magnitude and phase of the electric profile are changed which are easily distinguishable.

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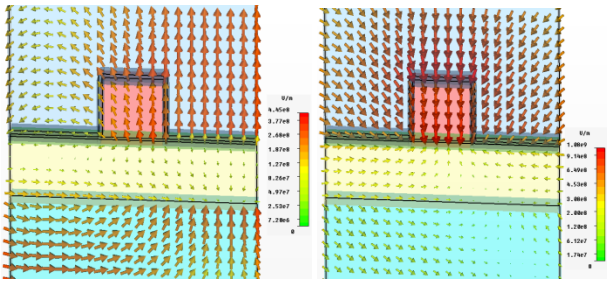

before detection after detection

Fig. 1. Illustration of electric field profile for the GG-SPRB before and after detection of biomolecules.

III. Modeling and Simulation

A schematic of the 3-D representation of the GG-SPRB with rectangular subwavelength grating geometry is shown in Fig. 2 which employs an array of periodic subwavelength dielectric grating onto the graphene layer. The incorporation of dielectric grating into the GG-SPRB supports the enhanced excitations of SPs and mediates the interactions between the excited SPs and the biomolecular layer on the sensing surface.

A laser beam is used to couple with a prism and which in further excite the SPs in the interface for matching the evanescent wave. The prism used in this simulation is fused silica glass and hence the corresponding dielectric constant and other parameters are taken into account from the reported article. The base of the prism is covered with a gold thin film of 50 nm and thereafter a sheet of 2 nm thick graphene layer is placed on top of the gold thin film. Finally, a periodic dielectric subwavelength grating is placed on top of the graphene layer. The thickness of the gold thin film is chosen as 50 nm. Whereas, the thickness of the graphene layer is selected as 2 nm. In this study, a dielectric material, polymethyl methacrylate (PMMA) is considered for the subwavelength grating with a dielectric constant of 2.25 [17]. The height (h_g), width (w_g), and period (P) of the grating is initially selected as 45 nm, 70 nm and 250 nm, respectively.

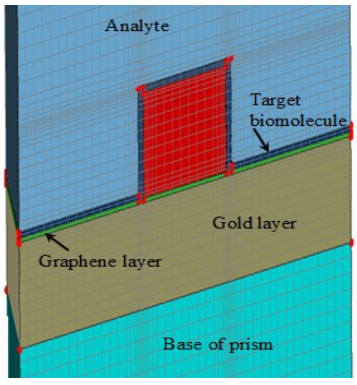

Fig. 2: 3-D model of the GG-SPRB having a rectangular grating geometry.

The outer surface of the dielectric grating is immobilized with ssDNA for the corresponding cDNA that recognizes and bind to the target cDNA. Target biomolecules from the sample analyte are diffused and captured by the receptor molecules. To excite the SPs, a TM-polarized plane wave light of fixed wavelength 632.8 nm is used. The light is coupled to prism with various incidence angles to find out the required coupling condition. The laser beam is reflected from the base of the prism and is normal to the surface. The reflected beam is directed to an optical detection system producing a SPR curve.

The structure under investigation is modeled and implemented with the help of the well-established FDTD and FEM methods in CST Microwave Studio. The refractive index (RI) profile and other properties of the examined materials are included in the simulation to analyze the performance parameters. The simulation study is verified with the theoretically developed formula based on the Fresnel equations and the matrix formalism. The simulator calculates the Fresnel coefficients of the layer system with recursion formalism. The properties of materials used in the modeling are assigned from the material database. In particular, the wavelength dependent complex valued RI of gold is assigned from the Drude model [18] from the material database. The RI of the fused silica glass prism is described by Sellmeier dispersion formula [19].

In order to get the plasmon resonance with photons both the wave vector and effective RI of the guided wave is altered as follows [20, 21]:

$$k_{sp}^{(m)} = k_{x,photon}\sin\theta_i \pm m\,k_{grating} = \frac{2\pi}{\lambda} n_p \sin\theta_i \pm m\frac{2\pi}{P} \quad (1)$$

and

$$n_{eff} = n_b \sin\theta_{res} \pm m\,\frac{\lambda}{P} \quad (2)$$

where, $k_{x,photon}$ and $k_{grating}$ are the wave vectors of an incident photon and grating respectively. $k_{sp}^{(m)}$ is the wave vector of surface plasmon polariton mode excited by the m^{th} order diffraction, P is the diffraction grating period and n_b is the RI of the cover media. For the sub wavelength grating-mediated interactions between SP and target bioanalytes, the following momentum matching relation is preserved:

$$k_{sp}^{(m)} = \frac{2\pi}{\lambda} n_p \sin\theta_{res} \pm m\frac{2\pi}{P} = \frac{2\pi}{\lambda}\sqrt{\frac{\varepsilon_M\,\varepsilon_{D,eff}}{\varepsilon_M + \varepsilon_{D,eff}}} \quad (3)$$

IV. Results and Discussions

As a quantitative measure of the sensor performance, detection sensitivity and accuracy are considered in the peak based detection method to indicate the detection information. Although, the biosensor is investigated for three different grating configurations, the biosensor with rectangular grating provides better performance.

It was demonstrated in our earlier study [22] that a graphene-based SPRB (G-SPRB) structure improves sensitivity. However, with the proposed GG-SPRB sensitivity is further improved compared with the G-SPRB. The modification of the G-SPRB to produce the GG-SPRB is accompanied by incorporating a periodic array of subwavelength grating on top of the layer of the graphene sheet.

In another study, the shift of the resonance peak angle with the GG-SPRB is compared for both the conventional

SPRB and the G-SPRB by considering the RI of the binding layer which increases in accordance with the concentration of target analytes. The summary of the investigation is shown in Fig. 3. The absolute analyte concentration considered in this simulation is equivalent to the RI of the resultant hybridization reaction. It can be seen from the figure that the GG-SPRB provides a larger shift as compared to both the conventional SPRB and the G-SPRB. Furthermore, the simulation results as produced by the FDTD allow us to obtain nearly ideal outputs that closely match the theoretical predictions (solid red line).

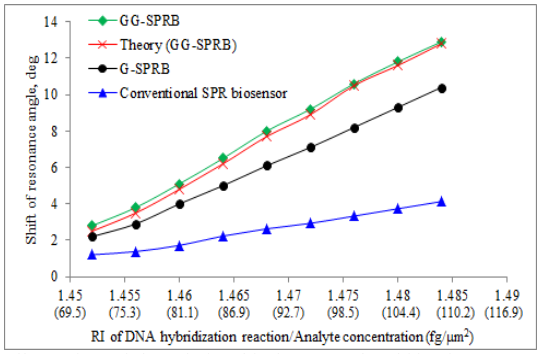

Fig. 3. Illustration of the relationship between the shift of resonance angle and the RI change for the GG-SPRB during the course of DNA hybridization.

The shift of resonance peak for the three grating configurations is compared in Fig. 4. It is obvious that both triangular and sinusoidal grating configurations in the GG-SPRB produce a slightly higher shift of the resonance peak angle. However, accuracy is significantly reduced by these two configurations since the resulted SPR curve broadens. It further decreases when the resonance peak condition shifted. To establish a relationship between the resonance peak angle (θ_{res}) and the SPR width ($\Delta\theta_{1/2}$), the resonance condition is modified by varying other design parameters (e.g., number graphene layer, thickness of biomolecular layer). Calculating $\Delta\theta_{1/2}$ for each θ_{res}, Fig. 5 is plotted for the GG-SPRB with rectangular grating configuration. An exponential curve fit is demonstrated. It is shown that the relationship between the SPR width and resonance angle is almost exponential.

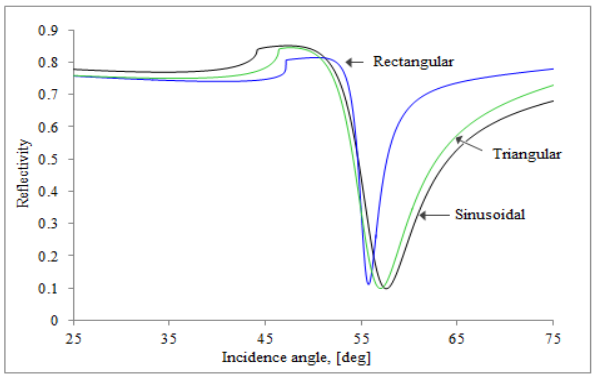

Fig. 4. Reflectivity versus incidence angle curve for rectangular, triangular and sinusoidal grating configurations in the GG-SPRB.

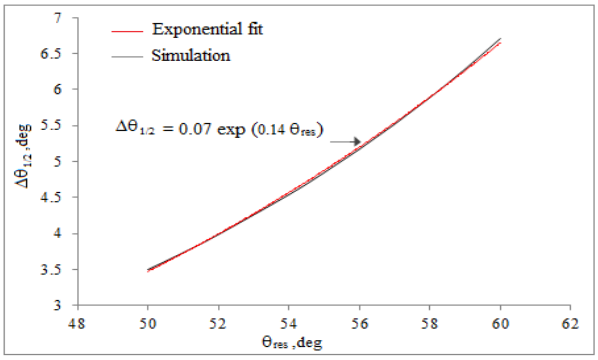

Fig. 5. Illustration of $\Delta\theta_{1/2}$ for various resonance incidence angles with rectangular grating configurations in the GG-SPRB.

The dependency of $\Delta\theta_{res}$ and SNR for the GG-SPRB is investigated for different number of graphene layers. The results of this investigation are compared with that of the G-SPRB. Although, improved performance is found in terms of the shift of resonance angle for both the G-SPRB and the GG-SPRB, the GG-SPRB produces lower response compared to the G-SPRB. As shown in Fig. 6, $\Delta\theta_{res}$ increases with the number of graphene layers for both the G-SPRB and the GG-SPRB, but it varies slowly for the GG-SPRB compared to the G-SPRB. On the other hand, it is shown in Fig. 6 (b) that SNR reduces with the number of graphene layers, however, it reduces slowly for the GG-SPRB compared to the G-SPRB.

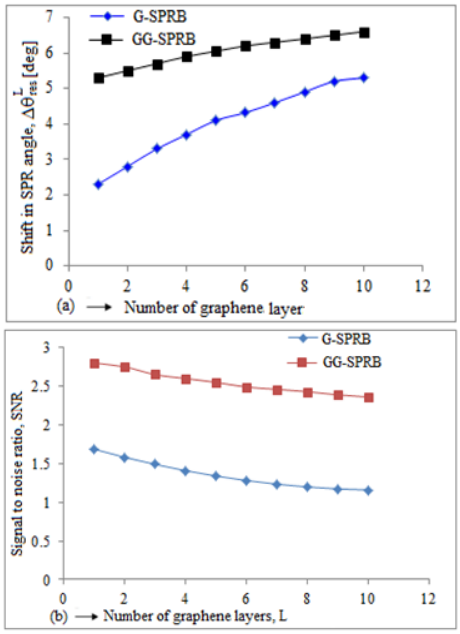

Fig. 6. Demonstration of the shift of resonance angle and SNR as a function of the number of graphene layers.

V. Conclusions

A computationally efficient method for the periodic array based GG-SPRB was presented for the DNA detection. Improved sensitivity is resulted from the incorporation of a graphene layer on top of the gold thin film together with the attachment of a periodic grating on

the graphene layer improved sensitivity. Compared with the conventional SPR biosensor and G-SPRB, a periodic array of subwavelength grating on a graphene layer produces large SPR signal amplification, which is the result of the excitations and coupling of bulk SPPs and SPs in the dielectric grating. Apart from its good performance, its greatest advantage is its tunable operation to achieve the desired permanence improvements by varying any of the design parameters.

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