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Fano resonance in graphene-MoS_2 heterostructure-based surface plasmon resonance biosensor and its potential applications

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ABSTRACT

We propose a new configuration of surface plasmon resonance (SPR) sensor that is based on graphene-MoS_2 hybrid structures for ultrasensitive detection of molecules. The present configuration is consisted of chalcogenide glass (2S2G) prism, Ag, coupling layer, guiding layer, graphene-MoS_2 heterostructure and analyte. We perform numerical and analytical study of the impact of the thickness and refractive index (RI) of the coupling and guiding layer in a planar sensing structure within the Kretschmann configuration on the resonance properties of the excitation. Results of reflectivity calculations clearly demonstrate the sharp Fano-type resonance appears in the curve of SPR because of the coupling between surface plasmon polariton (SPP) and planar waveguide (PWG) modes. The properties of the Fano resonance (FR) strongly depend on the parameters of the structure. The calculated magnetic field profiles manifest that the hybrid nature of the electromagnetic (EM) modes excited in the present structure. The proposed system displays an enhancement factor of sensitivity by intensity more than 2×10^3-fold when compared to the SPR sensing scheme.

1. Introduction

Surface plasmon-based sensors have enabled bio-molecular detection with high speed and sensitivity, which is mainly because they eliminate time-consuming labeling process and reduce molecular binding disturbance compared to common fluorescent optical sensors [1–3]. Surface plasmon resonance (SPR) sensors generally utilize the resonance excitation of surface plasmon polariton (SPP) at the metal-dielectric interface [4,5]. Among different kinds of SPR sensors, the most common one is the Kretschmann's configuration which is extensively used for chemical/biomolecular sensing with high sensitivity [6]. In such configuration, a thin metal film is deposited on a prism and the other face of the metal is kept in contact with the sensing medium. When a transverse magnetic (TM)-polarized incident light passes the prism through the metal film into a dielectric media, an evanescent wave will occur, while the energy of the incident light is absorbed and surface plasmon waves (SPWs) will be excited at the interface [7]. The SPR condition takes place at a specific angle of incidence or wavelength, when the evanescent wave couples with the SPs on the surface of the metal layer.

It is necessary to mention that the nature of the reflectance curve of attenuated total reflection (ATR) system dictates the performance of the SPR sensor. As such, the width of the SPR curve determines how precisely a sensor can detect the resonance angle and the shift. For high performance sensor, the shift in the resonance angle should be large, whereas the width of the SPR curve should be very small [8–10]. Different approaches for the improvement of the SPR sensor resolution have been proposed [11–13]. For example, high index coupling prism can be used to reduce the full width at half maxima (FWHM) of SPR curve thereby increasing the detection accuracy of the sensor [13]. Another way is choosing the metal layer correctly. Gold (Au) produces large SPR resonant angle shift while its response curve is relatively wider than that of silver (Ag). Au is usually preferred because it is more resistant to oxidation and corrosion in different environments. But, the drawback is that biomolecules adsorb poorly on gold, which limits the sensitivity of the conventional SPR biosensor. Aluminum (Al) not only exhibits narrower resonance curve compared to Au and Ag but also is relatively economical. However, Al is highly susceptible to oxidation, thereby deteriorating the sensor

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performance [14]. It has been shown that the use of bimetallic configuration (Au-Ag) increases the signal-to-noise ratio and decreases the width of the resonance curve, providing a significant improvement of the resolution while the sensitivity was comparable of that of conventional SPR [15–18].

To further improve the performance of biosensor, researchers have proposed and fabricated SPR based sensor coated with graphene layers [19–25]. Graphene is a single-atom thin planar sheet of sp_2 carbon atoms perfectly arranged in a honeycomb lattice. Graphene and graphene oxide provide good support for biomolecule adsorption due to their large surface area and rich π conjugation structure, making them suitable dielectric top layers for SPR sensing [23]. However, graphene produces more damping in SPs due to large imaginary dielectric constant for higher graphene layers, and hence results in decreased performance [24]. More recently, ultra-thin layer of molybdenum disulfide (MoS_2) that belongs to the transition-metal dichalcogenide (TMDC) semiconductor group is known as “beyond graphene” 2D nanocrystals material and they are widely used as solid lubricants due to its low friction property.

Therefore, in order to enhance the performance of conventional SPR sensor and utilize the advantageous properties of graphene, a planar structure of prism-waveguide coupling system with graphene-MoS_2 heterostructure that allows for coupling between SPP and WG mode is proposed. MoS_2 layers are used for improving the light absorption in order to provide enough excitation energy or effective charge transfer, while monolayer graphene is acting as io-recognition component for capturing the target biomolecules through pi-stacking force. We show that sharp Fano line shapes appear in the ATR spectra when the structural parameters are appropriately chosen. The thickness of the coupling and guiding layer is optimized first with respect to sensitivity, full width at half maximum (FWHM), and minimum reflectance at 633 nm wavelength. Thereafter the variation of performance parameters sensitivity, detection accuracy, quality factor, and minimum reflectance is shown with respect to the regular change in the RI of the sensing layer. The results of the numerical calculations clearly exhibit sharp Fano-type resonances, and demonstrate that the sensor sensitivity by intensity can be enhanced by more than 2×10^3 orders of magnitudes compared to that of conventional SPR sensors.

2. Design consideration and theoretical model

In our proposed new structure, a well-known Kretschmann configuration with multilayer thin films is employed. Multilayers are placed according to the following structure, i.e. 2S2G prism, Ag film, coupling layer, guiding layer, MoS_2, monolayer graphene and sensing medium, as shown in Fig. 1. The wavelength of the incident light for the excitation of SPs is 632.8 nm. The TM-polarized light incidents from one lateral face of the prism, then reaches to its base and totally reflected out from the other lateral face, and finally can be collected and analyzed by a photodetector.

2.1. Refractive index of various layer components

The first layer is 2S2G prism, and its refractive index (n_p) is calculated through the following relation [26]:

$$n_p = 2.24047 + \frac{2.693 \times 10^{-2}}{\lambda^2} + \frac{8.08 \times 10^{-3}}{\lambda^4} \tag{1}$$

where λ is the wavelength of incident light in micrometers. We choose 2S2G as the coupling prism due to its high refractive index. 2S2G also has shown potential in the fabrication of ultra-low-loss waveguides [27], and it has been widely used in sensing technology [28].

In the calculation, the dielectric function of metal is described by the Drude model as follows:

$$\varepsilon_{Ag}(\omega) = \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\gamma\omega} \tag{2}$$

where ε_∞ is the infinite frequency dielectric constant, ω_p is the bulk plasma frequency, ω is the angular frequency, and the collision frequency γ which is related to the dissipation loss in the metal. These parameters are set as 6.0, 1.5×10^{16} rad/s and 7.73×10^{13} rad/s, respectively [29]. The complex refractive index of monolayer MoS_2 at 632.8 nm is obtained from the experimental measurement data by Castellanos-Gomez et al. [30] and the thickness of MoS_2 layer is 0.65 nm [31]. The sixth layer in our model is monolayer graphene (with thickness of 0.34 nm) and its complex refractive index n_g in the visible range is given as [32]:

$$n_g = 3.0 + i\frac{C_1}{3}\lambda \tag{3}$$

where the constant $C_1 \approx 5.446\ \mu m^{-1}$ [33] and λ is the wavelength of incident light in μm.

The sensing medium for initial calibration is deionized (DI) water and its refractive index (n_s) is determined by the following relation [34]:

$$n_s^2 - 1 = \sum_{i=1}^{4} \frac{A_i \lambda^2}{\lambda^2 - t_i^2} \tag{4}$$

where the Sellmeier coefficients $A_1 = 5.666959820 \times 10^{-1}$, $A_2 = 1.731900098 \times 10^{-1}$, $A_3 = 2.095951857 \times 10^{-2}$, $A_4 = 1.125228406 \times 10^{-1}$, $t_1 = 5.084151894 \times 10^{-3}$, $t_2 = 1.818488474 \times 10^{-2}$, $t_3 = 2.625439472 \times 10^{-2}$, $t_4 = 1.073842352 \times 10^{1}$ and λ is the wavelength of incident light in μm. Eq. (4) is valid for wavelengths ranging from 0.182 to 1.129 μm.

2.2. Numerical formulation of reflectivity and field distributions

To systematically investigate the reflectivity change in our graphene-MoS_2 hybrid structure-based SPR sensing system, we employed the transfer matrix method (TMM) and Fresnel equations based on an N-layer model to perform a detailed analysis [13,19,20]. TMM method is a powerful tool in the analysis of light propagations through layered dielectric media. The central idea lies that electric or magnetic fields in one position can be related to those in other positions through a transfer matrix. Within the framework of the TMM [35,36], there are two kinds of matrices: one is the transmission matrix and the other is the propagation matrix. They connect the fields across an interface and the fields propagating over a distance within a homogeneous medium, respectively. For a stack of N dielectric layers shown in Fig. 1 (a), the transfer matrix can be obtained by transmission and propagation matrices across different interfaces and homogeneous dielectric media, respectively. In order to obtain the optical spectra, the equations which results from the ordinary boundary conditions that the fields satisfy at each interface need to be resolved. Since the system is uniform in the y direction, we can decompose the electromagnetic fields $\mathbf{E}^{(m)}$, $\mathbf{H}^{(m)}$ into two components and consider the TE and TM-polarized waves separately. And, the expressions of reflection and transmission coefficients for N-layer system (layer 0 corresponds to the prism and layer N to the analyte) is restated. For numerical calculations, it is assumed a planar multilayer slab sensor in Kretschmann configuration as schematically shown in Fig. 1 (c), where the