



Fano resonance in double waveguides with graphene for ultrasensitive biosensor

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Abstract: Fano resonance is realized in the multilayer structure consisting of two planar waveguides (PWGs) and few layer graphene, and the coupling mechanism between the two PWG modes with graphene is analyzed in detail. It is revealed that the Fano resonance originates from the different quality factors due to the different intrinsic losses of the graphene in the two waveguides, and the electric field distributions in the multilayer structure confirms our results. Fano resonance in our proposed structures can be applied in the ultrasensitive biosensor, and a significantly improved figure of merit (FOM) of 9340 RIU⁻¹ has been obtained by optimizing the structure parameters, which has a 2~3 orders of magnitude enhancement compared to the traditional surface plasmon polaritons (SPR) sensor. Especially, it is found that both transverse magnetic (TM)-polarization and transverse electric (TE)-polarization can support the Fano resonance, and hence it can work as ultrasensitive biosensor for both polarizations.

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References and links

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1. Introduction

Optical sensors have been extensively studied in recent years. Optical transducers, which are capable of detecting the minute changes in the refractive index, are widely used in the field of environmental monitoring [1,2], medical samples detection [3,4], food safety [5,6] and biochemical applications [7,8]. The reported optical sensing techniques include waveguide mode sensors [9,10], surface plasmon resonance (SPR) sensors [11,12], metasurface or metamaterials sensors [13] and etc. In waveguide sensors, evanescent waves in attenuated total

reflection (ATR) configuration are utilized to interact with the analyte. When light transmits in an optical waveguide, the optical field is not only distributed in the waveguide core, but also in the cladding. Therefore, the changes of refractive index in the cladding can be tracked by monitoring the transmission characteristics of the waveguide. Although intensive research has been carried out in waveguide sensors, hybrid configurations consisting of waveguides (such as Fano resonance) still attracts a lot of interests [14–17].

Fano resonance, whose asymmetry originates from the interaction of the broad resonance or continuum state with a narrow resonance or discrete state [18,19], were first discovered in quantum interference to describe asymmetric autoionization spectra of He atoms [20]. Although Fano resonance was originally introduced as a quantum-mechanical phenomenon, similar line shapes to Fano resonances were observed in various physical systems [21–23] and the classical models were well described with coupled harmonic oscillators [16,17]. In the past few years, researchers have made tremendous efforts to demonstrate the Fano line shapes in a variety of nanostructures, particularly in metamaterials and plasmonic nanostructures. Singh et al. realized Fano resonances at terahertz frequency through metamaterials or metasurfaces [24,25]. Lu et al. reported a waveguide-coupled resonators structure which can support Fano resonance [21]. Hayashi et al. realized a Fano resonance based on a waveguide-coupled traditional SPR structure [14]. Guo et al. designed a graphene/waveguide hybrid structure which is able to support Fano resonance at mid-infrared wavelength [15].

In the present paper, we found that a Fano resonance can be realized when two PWGs with different quality factors coupled together. The difference in quality factor between the two PWGs is caused by the intrinsic losses of graphene. Graphene, a two-dimensional material, has been extensively studied for its excellent electrical and optical properties such as its low loss and high field localization. It has been widely used in optoelectronic devices [26], solar cells [27], composite materials [28], biomedicine [29], and optical modulation [30,31]. It is well known that Fano resonance is excited by the coupling of a broad resonance and a narrow resonance. In this paper, a low quality factor waveguide is attached with graphene to generate a broad resonance. While another high quality factor waveguide provides an extra sharper resonance. The proposed Fano resonance can operate in both TM-polarized and TE-polarized modes, while the conventional SPR sensors can only operate in TM-polarized mode. We believe that the sharp asymmetric line shape characteristic of Fano resonance can find good applications in ultrasensitive biosensors.

2. Theoretical model and method

Figure 1(c) shows the proposed hybrid structure, which composes of two waveguides with graphene sheet. In PWG 1, as shown in Fig. 1(a), the graphene is attached on the waveguide layer, which has a small quality factor and generates a broad resonance. In PWG 2, as shown in Fig. 1(b), the graphene is covered on the cladding layer, which is far from the waveguide layer. As a result, PWG 2 can provide a sharp resonance due to its large quality factor. When these two waveguide modes are coupled together, a Fano resonance occurs as indicated in Fig. 1(c). SF10 with the refractive index $n_p = 1.723$ is chosen as the prism, which is used to excite the PWG mode. The cladding layers of the two PWGs are set to be cytop ($n_1 = n_3 = 1.34$). The core layers of the two PWGs are set to be ZnS-SiO₂ with $n_2 = n_4 = 2.198$. The sensing medium is set to be water ($n_s = 1.33$). The wavelength of the incident light is set to be 633nm. The thickness of core layer d_4 of the PWG 2 is fixed at 90nm. The thickness of cladding layer d_1 , d_3 and the thickness of core layer d_2 of the PWG 1 will be discussed and optimized in the next analysis.

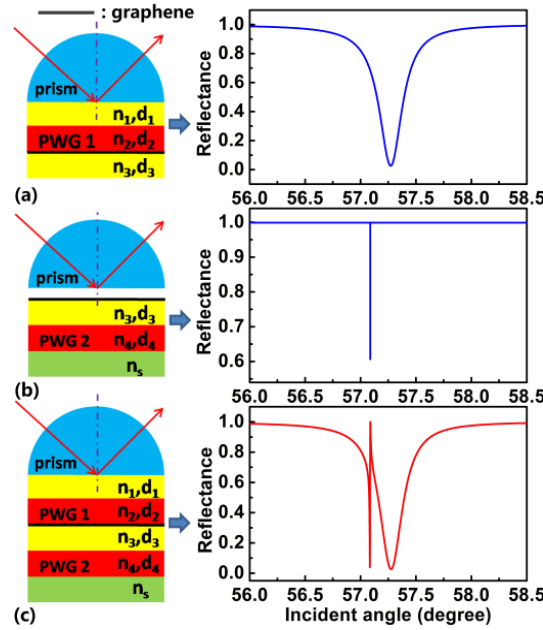


Fig. 1. Schematic diagram and the corresponding reflection spectra of (a) PWG 1, (b) PWG 2, and (c) proposed Fano resonance structure.

The effective refractive index is utilized to examine the condition for the coupling between the two PWG modes. Although the two PWG modes support both TM and TE modes, here only the TM mode is analyzed first. The dispersion relationship of PWG 1 with graphene can be derived as:

$$\tan h \alpha_2 d_2 = -\frac{\Gamma_1 + \Gamma_3}{1 + \Gamma_1 \Gamma_3} \quad (1)$$

with $\Gamma_1 = \alpha_2 \epsilon_1 / \alpha_1 \epsilon_2 (1 + i\sigma\alpha_1 / \omega\epsilon_1 \epsilon_0)$, $\Gamma_3 = \alpha_2 \epsilon_3 / \alpha_3 \epsilon_2$, and $\alpha_j = \sqrt{\beta^2 - k_0^2 \epsilon_j}$, $j = s, 1, 2, 3, 4$, β is the x component wavenumber, ϵ_j is the permittivity. ω is the frequency of the incident light. $\sigma = \sigma_{\text{intra}} + \sigma_{\text{inter}}$ is the conductivity of the graphene which is expressed using the Kubo formula [32,33]:

$$\sigma_{\text{intra}} = i \frac{e^2 K_B T}{\pi \hbar^2 (\omega + i\tau)} \left[\frac{E_F}{K_B T} + 2 \ln(e^{-\frac{E_F}{K_B T}} + 1) \right], \quad (2)$$

$$\sigma_{\text{inter}} = i \frac{e^2}{4\pi\hbar} \ln \left| \frac{2E_F - (\omega + i\tau)\hbar}{2E_F + (\omega + i\tau)\hbar} \right|, \quad (3)$$

where e is elementary charge, $\hbar$ is the reduced Plancks constant, K_B is the Boltzmann constant and the temperature $T = 300\text{K}$. In our work, the phenomenological relaxation time is assumed to be $\tau = 0.1\text{ ps}$. E_F is determined by $E_F = \hbar V_F \sqrt{\pi n}$, $V_F = 10^6\text{ m/s}$, n is the carrier density. It can be noted that the Fermi energy have little influence on the conductivity in visible frequency.

Similarly, the dispersion relationship of PWG 2 can be written as,

$$\tan k_{4z}d_4 = \frac{k_{4z}(p_3\alpha_3 + p_s\alpha_s)}{k_{4z}^2 - p_3\alpha_3p_s\alpha_s}, \quad (4)$$

where $p_j = \varepsilon_3 / \varepsilon_j$, $k_{4z} = \sqrt{k_0^2 \varepsilon_4 - \beta^2}$, hence we can plot the real part of effective refractive index by numerical calculation of Eqs. (1) and (4).

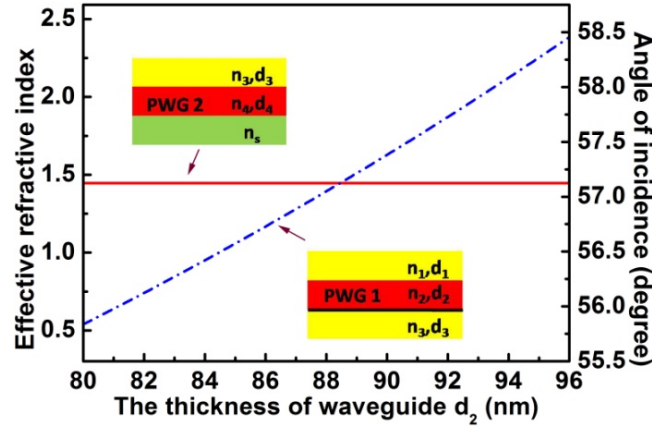


Fig. 2. Effective refractive indices of PWG 1 and PWG 2.

The effective refractive index for these two PWG modes, which is converted using the propagation constant ($n_{eff} = \beta / k_0$), are plotted as a function of d_2 in Fig. 2. The effective refractive index is determined by the position of the peak emerging in the reflection spectrum. The right ordinate represents the incident angle in the SF10 prism, where the incident light can excite the PWG modes with corresponding effective refractive index shown on the left ordinate. The red solid line in Fig. 2 is the effective refractive index of PWG 2 and its value is fixed at 1.446. The blue dash curve is the effective refractive index of PWG 1, which can intersect with red solid line at one point. The intersection point shows that the resonant angles of the two modes are in the same location, and hence the coupling between the two PWG modes is expected.

The transfer matrix method [34,35] for N -layer model are used to solve the multilayer systems. All layers of proposed structure stack along in the direction perpendicular to the prism. The arbitrary layer is defined by thickness d_k , dielectric constant ε_k , and refractive index n_k . The tangential fields at the first and the final boundary are set as $Z = Z_1 = 0$ and $Z = Z_{N-1}$, respectively, and their relation is given as:

$$\begin{bmatrix} U_1 \\ V_1 \end{bmatrix} = M \begin{bmatrix} U_{N-1} \\ V_{N-1} \end{bmatrix}, \quad (5)$$

where U_1 and V_1 are the tangential components of electric and magnetic fields at the boundary of first layer respectively. U_{N-1} and V_{N-1} are corresponding fields at the boundary of N th layer. M is the characteristic transfer matrix of the combined structure, and M is given as:

$$M = \prod_{k=2}^{N-1} M_k = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}, \quad (6)$$

with

$$M_k = \begin{bmatrix} \cos \beta_k & (-i \sin \beta_k)/q_k \\ -iq_k \sin \beta_k & \cos \beta_k \end{bmatrix}, \quad (7)$$

where $q_k = (\epsilon_k - n_k^2 \sin^2 \theta_{in})^{1/2} / \epsilon_k$, $\beta_k = 2\pi d_k / \lambda (\epsilon_k - n_k^2 \sin^2 \theta_{in})^{1/2}$ for TM-polarized mode, θ_{in} is the incident angle. We can get the amplitude reflection coefficient as:

$$r_p = \frac{(M_{11} + M_{12}q_N)q_1 - (M_{21} + M_{22}q_N)}{(M_{11} + M_{12}q_N)q_1 + (M_{21} + M_{22}q_N)}. \quad (8)$$

Finally, the reflectance (R_p) of N-layer model is given by

$$R = |r_p|^2 \quad (9)$$

3. Results and discussions

Figure 3(a) plots the ATR curves as a function of the incident angle (θ_{in}) of light beam in the prism, where the thickness of waveguide layer of PWG 1 varies from 90nm to 87nm. At $d_2 = 90\text{nm}$, as can be seen from the two reflection dips, both PWG modes are excited. However, the two dips are separated apart corresponding to the large difference in effective refractive index. It is known that mode coupling and Fano resonance are expected if the separation between these two PWG modes is reduced. For this reason, we reduce the thickness d_2 to 89nm, and as expected, when the two resonance modes are gradually approaching, the sharp asymmetric line shape of reflectivity can be observed. If the thickness d_2 is further reduced to 88nm, the approximate symmetric line shape of Fano resonance emerges which corresponds to the cross point predicted in Fig. 2. In this case, the coupling between the two PWG modes achieves its peak. This symmetry line shape can also be called electromagnetically induced transparency (EIT). EIT can be viewed as a special case of Fano resonance with symmetric line shape [18,19,36]. When the thickness d_2 is changed to 87nm, the line shape of reflectance is changed to be asymmetric again. To our knowledge, the sharp asymmetric line shape feature of Fano resonance is expected to find a good application in sensors. In the following discussion, the thickness of the waveguide above is set to 89nm for its sharp asymmetric line shape.

To explore the source of the Fano resonance further, the electric field (E) distribution inside the structure are calculated and plotted. The interface between the prism and cytop is set to be $Z = 0$. The normalized electric field by incident electric field (E_0) distributions in Fig. 3(b) and Fig. 3(c) are corresponding to the marked triangle and circle in Fig. 3(a). The triangle mark is located at the reflectance dip of waveguide mode of PWG 1 at the angle of 57.28° , the electric field is mainly limited to PWG 1. The inset in Fig. 2(b) indicates that another waveguide mode is also excited, but it is depressed. The circular mark is located at the reflectance dip of Fano resonance at the angle of 57.08° , where the electric field is greatly enhanced for both two waveguide modes. The results clearly demonstrate the coupling between the two waveguide modes excites the Fano resonance.

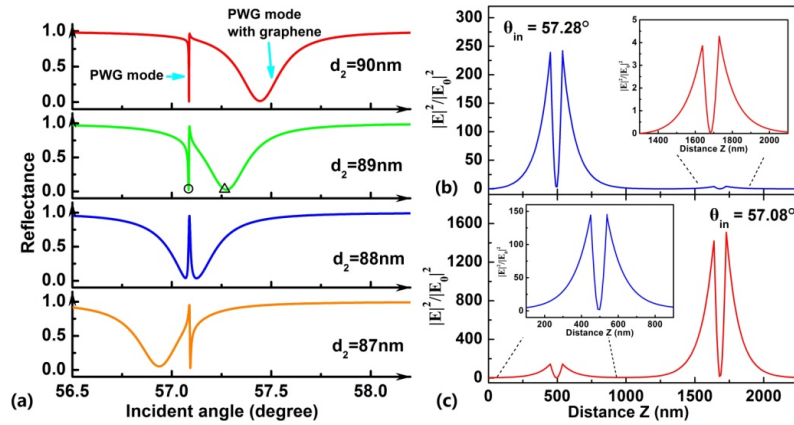


Fig. 3. (a) Reflectance as a function of the incident angle for different thickness d_2 . (b) Electric field profiles (field enhancement factors) with $d_2 = 89$ nm, $d_1 = 450$ nm and $d_3 = 1100$ nm for the triangular marks and (c) for the circular marks.

Due to the sharp asymmetric line shape characteristic of Fano resonance, the proposed structure has a great potential in ultrasensitive sensors application [14, 15, 17]. In the following analysis, the sensing mechanism using intensity modulation will be discussed. With the change of the refractive index in the sensing medium (dn_s), the reflectance is changed (dR) correspondingly. The sensitivity as a function of intensity can be derived as: $S_I(\theta) = dR(\theta)/dn_s$. The figure of merit by the sensitivity of the intensity, which is given by $FOM = \max_{\theta} |S_I(\theta)|$ [16, 17, 21], can be utilized to compare the sensitivity with different types of sensors.

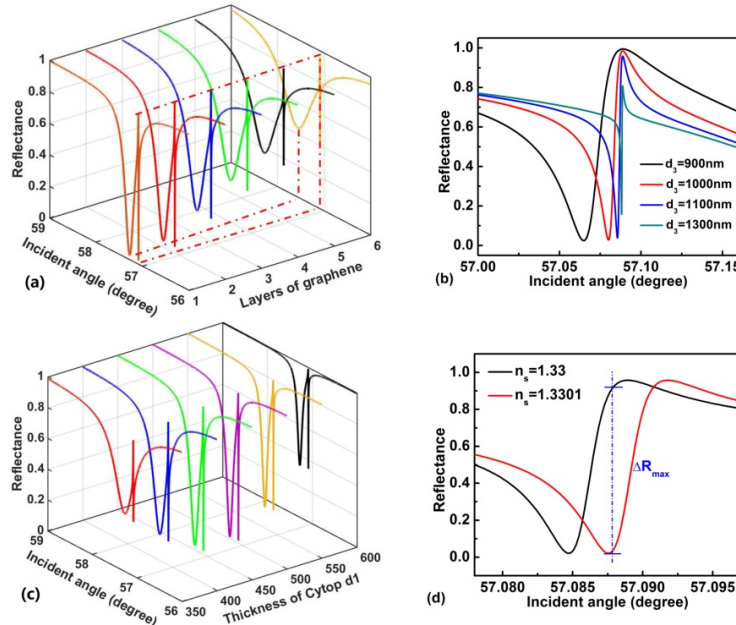


Fig. 4. (a) Reflectance as a function of the incident angle and the layer number of graphene; (b) Reflectance as a function of the incident angle for different thickness of coupling layer d_3 ; (c) Reflectance as a function of the incident angle and the thickness of cytop d_1 ; (d) The change of the reflectance dip in the multilayer thin films structure with the increase of the refractive index of water by 1.0×10^{-4} .

In order to improve the performance of the sensor, we have optimized the structural parameters of the proposed structure in Fig. 4. It is shown that the angular reflectance are dramatically influenced by the changes of the thickness of the PWG d_2 (Fig. 3(a)), and it is difficult to increase the sensitivity by controlling thickness of PWG in the laboratories. However, the asymmetric line shape of Fano resonance was found to have a significant effect on the sensitivity. The sensitivity can be fine tuned by the layers of graphene. In Fig. 4(a), a series of Fano ATR curves are showed with the changing of graphene layers. With larger number of graphene layers, the sensitivity increases due to an increase in asymmetry line shape of Fano resonance [37]. At the same time, the loss provided by graphene increases as well, which reduces the quality factor of two PWGs. Therefore, an optimal layer number exists, which is $L = 2$ in our proposed sensor.

Next, the dependence of sensitivity on the coupling layer thickness d_3 will be discussed to further improve the sensitivity. It is known that the steep part of the Fano line shape is utilized for sensing and the slope determines the sensitivity. Moreover, the radiation losses due to coupling between PWG and prism exist when PWG mode is excited by ATR method [38]. The quality factor of the PWG 2 can be increased with the increasing thickness of coupling layers, which will result in a narrower resonance. However, when the thickness continue to increase, the degradation of resonance will lead to a decreased sensitivity. There is an optimal value of d_3 , which is set to 1100nm in this work to get a higher sensitivity.

In Fig. 4(c), the Fano line shape is plotted with a series of thickness of cytop. When cytop is thin, the radiation losses have an more significant influence to the waveguide modes, such as, the quality factor of two waveguide becomes smaller and the resonance becomes broader. However, when thicker cytop is used, the quality factor of two PWG modes increase and the resonance is getting narrower, but the degradation of resonance will lead to the decreased sensitivity. To achieve the best sensitivity, the optimal thickness $d_1 = 425\text{nm}$ is used. Based on these optimized parameters, the sensitivities are calculated and shown in Fig. 4(d), where the sensitivity of 9340RIU^{-1} can be obtained.

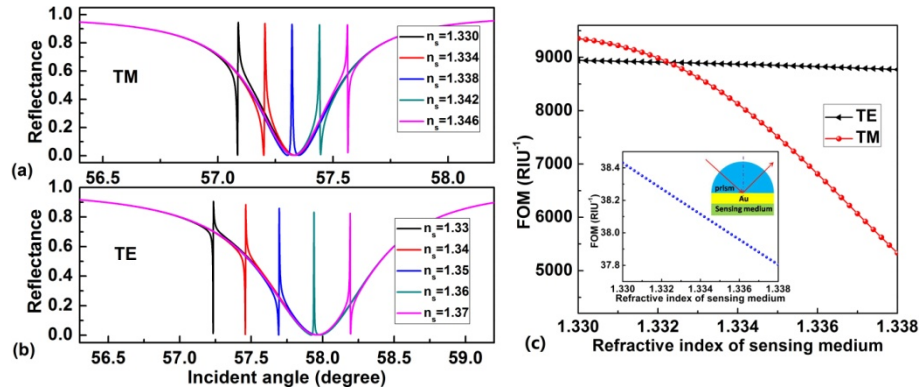


Fig. 5. Reflectance as a function of incident angle for different refractive index of sensing medium with (a) TM mode, (b) TE mode, where $d_1 = 340\text{ nm}$, $d_2 = 42\text{ nm}$, $d_3 = 1040\text{ nm}$, $d_4 = 40\text{ nm}$, and $L = 1$. (c) The dependence of FOM on the refractive index of sensing medium with both polarized modes, the inset shows the traditional SPR sensor based on 50 nm thick Au.

Figure 5(a) and 5(b) show the Fano line shape changed with the changing refractive index of sensing medium for the TM-polarized and TE-polarized modes, respectively. The sharp asymmetric Fano resonance is shifting to larger incident angle with an increasing refractive index of sensing medium for both polarizations. The Fano line shape becomes symmetry when $n_s = 1.338$ and $n_s = 1.36$ for TM-polarized and TE-polarized modes respectively. It is obviously that TE-polarized mode has a broader detection range. In Fig. 5(c), we compare the

FOMs of TM-polarized mode, TE-polarized mode and the traditional SPR sensor based on 50 nm thick Au. It shows that the FOM of TM-polarized mode is slightly higher than TE-polarized mode but the TE-polarized mode is more stable than TM-polarized mode when the refractive index of sensing medium increases. Compared to traditional SPR sensors, the proposed sensor achieves a significantly improved FOM, which is enhanced by 2~3 orders of magnitude.

4. Conclusions

In this paper, a prism coupled two waveguide structures are proposed to achieve a Fano resonance line shape in the reflection spectra. The loss from the graphene provides different quality factors for the two waveguides in the structure. The waveguide that has a smaller quality factor supports the broad resonance, while the other waveguide with a higher quality factor generates the sharp resonance. By coupling these PWG modes, a Fano resonance can be generated. The coupling mechanism between the two PWG modes are discussed in detail. When it is utilized in biosensors, both TM and TE modes presents an improved FOM by which is enhanced by 2~3 orders of magnitude compared to the traditional SPR sensor. We believe that the proposed designs can find good applications in optical sensing technology.

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