Independently tunable triple Fano resonances in plasmonic waveguide structure and its applications for sensing

Qiaohua Wu, Yingqiu Zhang, Desheng Qu, and Chunlei Li*
Northeast Forestry University, College of Science, Harbin, China

Abstract. A surface plasmon polaritons (SPPs) waveguide structure composed of a metal–insulator–metal waveguide with a baffle, a special square cavity (SSC), and a ring cavity (RC), is proposed to realize independent tuning in triple Fano resonances. Using the finite element method, the magnetic field distributions and optical transmission spectra of the structure are analyzed in detail. The simulation results show that the structure achieves triple Fano resonances originated from two different mechanics. One of Fano resonances occurs in the RC, and the others occur in SSC. By regulating the structure parameters of the SSC and RC, these Fano resonances can be well tuning, and independently tuning is realized in multiple Fano resonances, which provides flexibility for the structure to be applied to optical devices. In addition, the structure exhibits great performances in refractive index sensing and biosensing. The maximum sensitivity of refractive index sensing achieves 2350 nm/RIU, and there is a good linear relationship between resonance wavelength and refractive index. Due to great sensitivity and independent tunability, the SPPs waveguide structure may be potentially used in micronano-optical devices, especially in optical on-chip sensor. © 2022 Society of Photo-Optical Instrumentation Engineers (SPIE) [DOI: 10.1117/1.JNP.16.036008]

Keywords: surface plasmon polaritons; Fano resonance; independently tunable; sensing.

1 Introduction

Surface plasmon polaritons (SPPs) are evanescent waves that propagate along a metal–insulator interface. Those can break through the optical diffraction limit and confine the energy in deep-subwavelength dimensions, rendering them prospective for application in miniaturized optical devices. In recent years, a large number of optical devices based on SPPs have been proposed. Fano resonances can ubiquitously occur in a large variety of resonators. Among them, the SPPs waveguide structure based on Fano resonance has attracted extensive attention of researchers owning to the sharp asymmetric transmission peak. In the SPPs waveguide structure, Fano resonance is formed by coupling of local discrete states and broad continuous states. Unlike Lorentz resonance, the transmission spectrum of Fano resonance shows sharp and asymmetric transmission peaks. Meanwhile, the SPPs waveguide structure based on Fano resonance is sensitive to the refractive index of insulator. Thus, it is widely used in the field of micronano-optical sensing.

Compared with single Fano resonance, multiple Fano resonances are beneficial in biochemical sensing, refractive index sensing, and concentration detection. Multiple Fano resonances are becoming more and more important, and intense efforts have been devoted to achieve multiple Fano resonances. Liu et al. proposed a refractive index sensing structure based on double Fano resonance and discussed its application in hemoglobin concentration detection. Xu et al. reported a nanosensor with high refractive index sensitivity based on double Fano resonances. The application in temperature sensing and glucose concentration detection was exhibited. Fang et al. realized multiple Fano resonances in an end-coupled metal–insulator–metal...
(MIM) waveguide system, which gained high figure of merit (FOM) and high sensitivity. However, owing to the multiple Fano resonances are usually triggered by the collective behavior of the whole SPPs systems, it is hard to achieve independent tunability for multiple Fano resonances. The research should pay more attention to increasing the flexibility of device fabrications and the manipulation of optical transmission.

In this paper, independently tunable triple Fano resonances are realized in a designed SPPs waveguide structure that is composed of two independent resonators [special square cavity (SSC) and ring cavity (RC)] coupled with a bus waveguide. By changing the structure parameters, triple Fano resonances are tunable, and independently tuning is realized in multiple Fano resonances. Its application as a refractive index sensor is discussed; the highest refractive index sensitivity is up to 2350 nm/RIU. Based on the refractive index sensing, the structure can also be used for glucose concentration detection, and the maximal sensitivity of glucose concentration detection is 0.266 nm/(g/L). The structure’s performance benefited from the independent tuning ability of multiple Fano resonances and high refractive index sensitivity, the structure has significant potential applications in the field of integrated micronano-optical sensing.

2 Structure and Theory

Figure 1 shows a schematic diagram of the designed MIM waveguide structure, which consists of a bus waveguide with baffle, SSC, and RC. The MIM waveguide structure can be fabricated with lithography and deposition method. A sufficiently thick silver layer is deposited on the substrate by vapor deposition method, then the bus waveguide with baffle, SSC, and RC are etched on the silver layer. The white and gray parts denote insulator and silver, respectively. The SSC consists of a circle with the radius of \( R \) and a square with the side length of \( 2R + 2d \), \( d \) represents minimum width in the SSC. The inner and outer radii of the RC are \( r_1 \) and \( r_2 \), respectively. Therefore, the effective radius of the RC can be defined as \( r = (r_1 + r_2)/2 \). A baffle was set in the middle of the MIM waveguide and the thickness of the baffle is fixed at \( t = 10 \) nm. The width of bus waveguides and RC are fixed at \( w = 50 \) nm to ensure that only one fundamental transverse magnetic (TM0) can exist and propagate.
For TM0 mode, the dispersion relationship of SPPs in MIM waveguide can be expressed as

\[ \varepsilon_i \sqrt{\beta^2 - \varepsilon_m k_0^2} + \varepsilon_m \sqrt{\beta^2 - \varepsilon_i k_0^2} \tanh \left( \frac{\sqrt{\beta^2 - \varepsilon_i k_0^2}}{2} \right) = 0, \quad (1) \]

where \( \beta \) represents the propagation constant of SPPs, \( k_0 \) represents the wave vector in vacuum, \( \varepsilon_m \) and \( \varepsilon_i \) represent the relative dielectric constant of silver and insulator, respectively. The value of \( \varepsilon_m \) can be calculated by Drude model:

\[ \varepsilon_m(\omega) = \varepsilon_\infty - \frac{\omega_p^2}{\omega(\omega + i\gamma)}, \quad (2) \]

where \( \varepsilon_\infty = 3.7 \) is the relative dielectric constant at infinity, \( \omega_p = 9.1 \) eV is the plasma frequency, \( \gamma = 0.018 \) eV represents the loss of metallic silver, and \( \omega \) represents angular frequency of incident wave.

When the incident SPPs propagates along the \( x \) axis in the waveguide, parts of them can couple into the resonant cavity and generate phase change. When the phase-match condition is satisfied, resonance phenomenon will appear. The resonance wavelength (\( \lambda_{\text{res}} \)) can be described as

\[ \lambda_{\text{res}} = \frac{L_{\text{eff}} n_{\text{eff}}}{m}, \quad (3) \]

where \( L_{\text{eff}} \) is the effective length of the resonant cavity, \( m \) is resonance mode order, and \( n_{\text{eff}} \) represents the real part of effective refractive index and can be calculated as \[ n_{\text{eff}} = \text{Re}(\beta/k_0). \]

The propagation properties of the SPPs are analyzed by the finite element method. The perfect matching layers are set at each boundary of the simulation area to absorb the escaping electromagnetic waves. The fine triangular meshes are selected to ensure the convergence and accuracy of the simulation results, and the maximum triangular mesh size is 10 nm.

3 Results and Discussion

3.1 Formation Mechanism of Fano Peaks

To investigate the optical properties of the structure, the transmission spectra of the structure without baffle, the MIM waveguide with baffle, and the whole structure are shown in Fig. 2. The geometric parameters of the structure are set as \( r = 205 \) nm, \( R = 180 \) nm, \( d = 20 \) nm,
and $g = 10\ \text{nm}$. For the structure without baffle, as shown in the red line, there are three transmission dips at 1390, 1800, and 2235 nm in the transmission spectrum, which can be treated as narrow discrete states. Meanwhile, the MIM waveguide with baffle can form a broad continuum state as shown in the black line. For the whole structure, as a result of the interference of the discrete states and the continuum state, there are three Fano peaks (FR1, FR2, and FR3) at the wavelengths of 1364, 1790, and 2222 nm, as shown in the green line.

To further understand the mechanism of Fano resonances of the designed structure, the magnetic field distributions ($H_z$) at the resonance wavelengths are simulated as shown in Fig. 3. It can be seen that the energy is almost distributed in the SSC at the wavelengths of 1364 and 2222 nm. On the contrary, most of the energy is distributed in the RC at the wavelength of 1790 nm. This phenomenon indicates that both FR1 and FR3 may be more affected by SSC, and the RC may have more powerful effect on FR2. The two magnetic field distributions of FR1 and FR3 show that the SPPs coupled into SSC meet the resonance conditions, and the resonance mode orders at FR1 and FR3 are 2 and 1, respectively. Figure 3(b) shows that the SPPs in RC produce a phase shift of $2\pi$ and the resonance mode order is 1.

### 3.2 Tunable Fano Resonance and Its Applications for Sensing

First, we investigate the influences of the SSC and RC sizes on Fano resonances of the structure. In Fig. 4(a), the inner radius $R$ of SSC increases from 180 to 200 nm in step of 5 nm, and the structural parameter $d$ is fixed at 20 nm. The approximately linear relationships between the...
resonance wavelengths and the inner radius of the SSC are shown in Fig. 4(b). When the structure parameter $R$ increases from 180 to 200 nm, the wavelengths of FR1 and FR3 are increased by 100 and 230 nm, respectively, but FR2 keeps unchanged. Analyzing of these results, FR1 and FR3 meet the resonance conditions in SSC, while FR2 meets the resonance conditions in RC. According to Eq. (3), only changing the size of SSC will change the wavelengths of FR1 and FR3, while that of FR2 remains unchanged. Figure 5(a) shows the transmission spectra for different effective radii of the RC from 205 to 235 nm with step of 10 nm, and the linear fitting curves between the resonance wavelengths and the effective radius of the RC are shown in Fig. 5(b). As the effective radius $r$ increases, the wavelength of FR2 increases from 1790 to 2048 nm, and those of FR1 and FR3 remain unchanged. This phenomenon shows that the size of RC only affects FR2. Therefore, FR1 and FR3 can be tuned by changing the structural parameter $R$ of the SSC, while FR2 can be tuned by changing the effective radius of the RC. Independent tuning in multiple Fano resonances is realized.

Successively, we investigate the effect of the refractive index of the insulator in the resonators on the position of Fano resonance peaks. The refractive indexes of the insulator in the SSC and RC increases from 1.0 to 1.12 with a step of 0.04, and the other area refractivity remains unchanged. The corresponding transmission spectra are exhibited in Fig. 6(a). It can be seen that the resonance wavelengths of the triple Fano resonances appear obvious redshifts and the Fano resonances are sensitive to the insulator refractive index of the resonators. The phenomenon can be explained by Eqs. (1)–(3). With the increase of the refractive index of the insulator in...
the SSC and RC, the effective refractive index increases, and then the resonance wavelength redshifts. Figure 6(b) shows the linear fitting relationships between the resonance wavelengths of the three Fano peaks and the refractive index of the insulator in the SSC and RC. It can be seen that FR1, FR2, and FR3 have good performances in linearity. The linear correlation coefficients of FR1, FR2, and FR3 are 0.99992, 0.9993, and 0.99995, respectively.

Based on the linear adjustment of Fano resonance by refractive index of insulator, the designed SPPs waveguide can be used for the refractive index sensing. As an important index for evaluating sensing performance, sensitivity is defined as

\[ S = \frac{\Delta \lambda}{\Delta n}, \]

where \( \Delta n \) is the change of the refractive index of the insulator in the resonant cavities, and \( \Delta \lambda \) is the variation of the corresponding resonance wavelength. Therefore, the refractive index sensitivities of FR1, FR2, and FR3 can be expressed by the slope of the fitting lines in Fig. 6(b). Those are 1330, 1785, and 2235 nm/RIU, respectively. It can be seen that FR3 has the largest sensitivity compared with FR1 and FR2. For the same dielectric properties of material for RC and SSC, FR3 has the greater sensitivity due to its higher resonance wavelength.37 In addition, another key factor to sensing performance is FOM, which is defined as

\[ \text{FOM} = \frac{\Delta T}{T \Delta n}; \]

where \( T \) represents the transmittance and \( \Delta T \) represents the transmittance change. The structure parameters are the same as the initial values. The FOM values at different wavelengths are shown in Fig. 7. It can be seen that the highest FOM reaches 3387 at 2395 nm. This result shows that the Fano peak is very sharp, which is conducive to the accurate measurement of the peak position.39

Based on the refractive index sensing performance, the SPPs waveguide structure is suitable for detecting biological parameters that have definite correlation with refractive index, such as the glucose solution concentration. The refractive index of glucose solution can be expressed as

\[ n_{\text{glucose}} = 1.1889 \times 10^{-4}C + 1.33230545, \]

where \( n_{\text{glucose}} \) is the refractive index of solution, \( C \) represents the concentration of glucose solution. In Fig. 8(a), the concentration of glucose solution in the SSC and RC increases from 0 to 400 g/L with a step of 100 g/L. According to Eq. (4), the refractive index of the resonators can be calculated. The simulation results show that the resonance wavelengths of the triple Fano resonances exhibit redshifts with the increase of solution concentration. The linear fitting relationships between resonance wavelengths and solution concentration are shown in Fig. 8(b). The slope of fitting straight lines of FR1, FR2, and FR3 are 0.164, 0.214, and 0.266, respectively. The linear correlation coefficients of FR1, FR2, and FR3 are 0.99921, 0.99965, and 0.99977, respectively. Exploiting the equation \( S_{\text{glucose}} = \frac{\Delta \lambda}{\Delta C} \), the calculated sensitivities of glucose solution sensing for FR1, FR2, and FR3 are 0.164, 0.214, and 0.266 nm/(g/L), respectively. The results show that all Fano peaks of the proposed structure can be used for glucose concentration sensing. The sensitivity of FR3 is higher than that of the other two Fano resonances, but the transmittance is lowest. The sensitivity of FR1 is lower than that of others, yet the transmittance is highest.
The sensitivity and transmittance of FR2 are between those of the other two. Thus, based on the need of sensitivity or transmittance, the appropriate Fano peak can be selected for glucose concentration sensing. It may provide flexibility for the application of this structure in sensing.

4 Conclusions

In summary, triple Fano resonances are realized in a proposed SPPs waveguide structure that consists of two different resonators and an MIM waveguide with baffle. By adjusting the inner radius of the SSC or the effective radius of the RC, the tunable triple Fano resonances is realized and the FR2 can be well tuned independently. Furthermore, the structure can be used for refractive index sensing with a great sensitivity of 2235 nm/RIU and a high FOM of 3387. Based on great sensitivity, the structure for detecting glucose concentration can realize the maximal sensitivity of 0.266 nm/(g/L). These results show the structure may be applied in high-performance optical integrated sensing devices.

Acknowledgments

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Fig. 8 (a) Transmission spectra at different concentrations of glucose solution. (b) Linear fitting between resonance wavelength and solution concentration.
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