Dynamically tunable Fano resonance with high Q factor based on asymmetric Dirac semimetal split-ring structure

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Abstract

We propose an asymmetric split-ring (ASR) structure based on Dirac semimetal, which has Fano resonance with a high quality (Q) factor in the terahertz (THz) band, the Q factor can reach a maximum value of 20.19. Amplitude modulation can be achieved by increasing the degree of asymmetry $\Delta \theta$ of the asymmetric split ring. As a result, in this study, an amplitude modulation of 27.19% has been achieved by increasing the asymmetry from $10^\circ$ to $40^\circ$. Furthermore, our full-wave electromagnetic simulations show that the frequency sensitivity values of Fano and quadrupole resonance are as high as 0.6 THz/refractive index unit (RIU) and 0.933 THz/RIU, respectively. In addition, the sensing range can be adjusted by changing the Fermi levels of Dirac semimetal. Our study can guide the practical application of ultrasensitive THz sensors.

1. Introduction

The Fano resonance is caused by the coherent coupling and interference between continuous and discrete states [1, 2]. Unlike the Lorentz resonance, the Fano resonance has a sharp and asymmetric line shape. Fano resonance, because of its narrow linewidth and high Q factor, can be used in biological and chemical sensors, waveguide modulators, optical switch, and slow light field [3–10], which resulted in gathering people’s attention related to research [11–15]. To date, various metamaterial structures, ranging from microwave to optical frequencies, based on Fano resonance have been proposed. For instance, Singh R et al obtained Fano resonance with a Q factor of up to 50 in the terahertz (THz) band by changing the asymmetry of the aluminum split ring [16]. Wen et al proposed a plasma nanometer sensor that uses Fano resonance based on the metal-insulator-metal waveguide structure [17]. Liu et al studied the optical properties of double-crossed nanowires, which exhibited Fano resonance in the near infrared region [18]. However, its applications have the following constraints: high metal loss, low modulation range, and complex permittivity functions. To avoid the constraints, two-dimensional (2D) materials like graphene are introduced in the field of sensing. Xia et al proposed a both graphene pattern and complicated bias gate free method to demonstrate the excitation and modulation of the graphene surface plasmons (GSPs) in a graphene monolayer [19], and the highest sensitivity of 1.77 $\mu$m/RIU and 2.3 $\mu$m/RIU are obtained, respectively. They also discuss more possibilities of anisotropic 2D materials beyond anisotropic response by using vertically stacked nanostructures (NSs) to achieve polarization-independent optical absorption in a pure anisotropic region [20]. The sensitivity of 2.43 $\mu$m/RIU and 2.08 $\mu$m/RIU has been obtained, respectively.

Three-dimensional (3D) Dirac semimetals are also a 3D analog of graphene, which is a new quantum matter discovered recently. 3D Dirac semimetals as the 3D analog of graphene have all advantages of graphene as that of photosensitive devices. 3D Dirac semimetals exhibit ultrahigh mobility that reaches $9 \times 10^5$ cm$^2$/V·s at 5 K [21], which is higher compared to graphene ($2 \times 10^5$ cm$^2$/V·s at 5 K) [22], because of their crystalline symmetry protection against gap formation [23–27]. Most importantly, Dirac semimetals can also dynamically control their surface conductivity by altering the Fermi energy. Chen et al introduced and segregated this
material into two parallel strips to construct plasmon-induced transparency (PIT) metamaterials (MMs) and obtained novel PIT optical responses by using the weak hybridization between the two strips. Therefore, it will be interesting to incorporate Dirac semimetals in the design of MMs to achieve dynamically tunable Fano resonance for sensing applications.

In this paper, we propose a two-gap THz asymmetric split-ring (ASR) structure based on Dirac semimetal films (DSFs). Fano resonance with a high Q factor transpires from a gentle symmetry-breaking structure. The Q factor of Fano resonance can be as high as 20.19, and the Q factor of quadrupole resonance can be as high as 22.19. Amplitude modulation can be achieved by increasing the degree of asymmetry $\Delta \theta$ of the asymmetric split ring. In this study, an amplitude modulation of 27.19% has been achieved by increasing the asymmetry from 10° to 40°. Moreover, the sensitivity values of Fano and quadrupole resonance of our designed resonator can reach 0.6 THz/RIU and 0.933 THz/RIU, respectively. Mainly, the sensing range of Fano and quadrupole resonance of the designed structure can be controlled by altering the Fermi energy. Our study has implications in various potential applications, such as, biological and chemical sensors, switches, and other THz devices.

2. Structural and method

Figures 1(a) and (b) depict the structure of the Fano resonator. The unit cell structure comprises a two-gap split ring deposited on the top of the SiO$_2$ substrate with a relative permittivity $\varepsilon$ of 3.9. The split ring is made of DSFs with a thickness of 0.2 $\mu$m. Unit cells are arranged in an array with a periodic length of $P_x = P_y = 6 \mu$m. The outer radius (R) and the width (w) of the split ring are 2.4 $\mu$m and 0.6 $\mu$m, respectively. The structure of ASR is shown in figure 1(a); the upper arcs span an angle of 170°, and the lower arcs span an angle of 150°. In addition, the upper and lower arcs of the symmetrical split ring (SSR) structure span an angle of 160°.

According to the random phase theory, the complex surface conductivity of a Dirac semimetal can be obtained by the Kubo formula. Considering the contribution of intraband and interband processes, the conductivity can be expressed as [27]:

$$\text{Re} \sigma(\Omega) = \frac{e^2}{h} \frac{g k_F}{24\pi} \Omega G(\Omega/2)$$

$$\text{Im} \sigma(\Omega) = \frac{e^2}{h} \frac{g k_F}{24\pi} \left[ \frac{4}{\Omega} \left( 1 + \frac{\pi^2}{3} \left( \frac{T}{E_F} \right)^2 \right) \right]$$

$$+ 8\Omega \int_{0}^{\infty} \left( \frac{G(\varepsilon) - G(\Omega/2)}{\Omega^2 - 4\varepsilon^2} \right) \varepsilon d\varepsilon$$

where $G(E) = n(-E) - n(E)$ with $n(E)$ being the Fermi distribution function, $k_F = E_F / h v_F$ is the Fermi momentum, $E_F$ is the Fermi energy, $v_F = 10^6$ m s$^{-1}$ is the Fermi velocity, $\varepsilon = E / E_F$, $\Omega = h \omega / E_F$, $\varepsilon_c = E_c / E_F$, $E_c$ is the cutoff energy, and g is the degeneracy factor. Correspondingly, the permittivity of 3D Dirac semimetals can be obtained by using the two-band model [27]:

$$\varepsilon = \varepsilon_b + i \sigma / \omega \varepsilon_0$$

where $\varepsilon = 1$ for $g = 40$ (for AlCuFe quasicrystals [29]) and $\sigma_0$ is the permittivity of vacuum. Fano resonator is modeled and studied by CST microwave studio frequency domain method. In the calculation, the unit cell boundary conditions in the x–y plane and Floquet ports in the z direction have been adopted. Plane waves are incident perpendicular to the metamaterial surface.
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when and the corresponding Q factor decreases gradually. An amplitude modulation of 27.19% has been achieved

the coupled Lorentz oscillator model and analyze it in combination with an electric

where x_{1} and x_{2} are the amplitudes, damping rates and effective mass of the

distribution at the frequencies of 5.63 THz and 8.85 THz is similar to that of dipole resonance in SSR, so it is also

similar to the upper arc and decreasing the central angle \( \theta \). As shown in figure 4, the resonance intensity and bandwidth increase with the increase of \( \Delta \theta \), and the corresponding Q factor decreases gradually. An amplitude modulation of 27.19% has been achieved when \( \Delta \theta \) has been increased from 10° to 40°.

To verify the asymmetric resonance of the structure and understand its inherent mechanism, we introduce

next, we introduce the degree of asymmetry (\( \Delta \theta = \theta_{1} - \theta_{2} \)) by increasing the central angle (\( \theta_{1} \)

corresponding to the upper arc and decreasing the central angle (\( \theta_{2} \)) corresponding to the lower arc. The Fermi

level of DSFs has been set at 90 meV, and the effect of different degrees of asymmetry on Fano resonance has

been discussed. As shown in figure 4, the resonance intensity and bandwidth increase with the increase of \( \Delta \theta \),

and the corresponding Q factor decreases gradually. An amplitude modulation of 27.19% has been achieved when \( \Delta \theta \) has been increased from 10° to 40°.

To verify the asymmetric resonance of the structure and understand its inherent mechanism, we introduce

the coupled Lorentz oscillator model and analyze it in combination with an electric field \([31, 32]\):

\[
\dot{x}_{1}(t) + \gamma_{1}x_{1}(t) + \omega_{0}\gamma x_{1}(t) + \kappa^{2}x_{2}(t) = g_{1}E_{0}/m_{1}
\]

\[
\dot{x}_{2}(t) + \gamma_{2}x_{2}(t) + (\omega_{0} + \delta)^{2}x_{2}(t) + \kappa^{2}x_{1}(t) = g_{2}E_{0}/m_{2}
\]

where \( x_{1} \) and \( x_{2} \), \( \gamma_{1} \) and \( \gamma_{2} \), and \( m_{1} \) and \( m_{2} \) represent the amplitudes, damping rates and effective mass of the

bright and dark modes, respectively. \( \omega_{0} \) and \( \omega_{0} + \delta \) are the resonant frequencies of the bright and dark modes,

respectively, and \( \kappa \) and \( \delta \) are the coupling coefficients of the two modes and the shifts of the resonant frequency,
respectively. \( g_1 \) and \( g_2 \) are the geometric parameters indicating the coupling strength of the bright and dark modes in the \( E_0 \) field. By solving (4) and (5), we can obtain the polarization of the metamaterial,

\[
\chi_{\text{eff}} = \frac{P}{\varepsilon_0 E_0}
\]

where \( P \) is the polarization intensity and \( \varepsilon_0 \) is the vacuum permittivity. As the Q factor is large, and the incident field interaction is weak, we assume that \( g_2 \) is zero. The EIT transmission in the THz region can be expressed as [33]:

\[
|T| = \left| \frac{4\sqrt{\chi_{\text{eff}} + 1}}{(\sqrt{\chi_{\text{eff}} + 1} + 1)^2 - (\sqrt{\chi_{\text{eff}} + 1} - 1)^2 e^{-\frac{2\pi d}{\lambda_0 \sqrt{\chi_{\text{eff}} + 1}}}} \right|
\]

where \( \lambda_0 \) is the wavelength in vacuum and \( \chi_{\text{eff}} \) is the effective susceptibility of the metamaterial structure. Figures 3(a) and (b) are simulated and fitted transmission curves with different degrees of asymmetry, respectively. The fitted curve and the simulated curve are roughly consistent. The result verifies the validity of the model structure. Table 1 shows the change of coupling coefficient with the increase of \( \Delta \theta \). It can be observed that \( \kappa \) is proportional to \( \Delta \theta \), which determines the modulation intensity of Fano resonance. In addition, the damping factors \( \gamma_1, \gamma_2 \) correspond to the decay rate in the atomic physics, which is inversely proportional to the spectral

Figure 3. (a)–(f) The electric field distribution at resonant frequency corresponding to figures 2(a) and (b) labelled A, B, C, D, E, F, respectively. The Fermi level of DSFs is 90 meV.

Figure 4. Fano resonance transmission spectra with different asymmetries.
linewidth. We observe that $\gamma_1$ and $\gamma_2$ are inversely proportional to $\Delta \theta$, which indicates that the coupling of bright mode and dark mode leads to the excitation of dark mode and the appearance of Fano resonance, and the resonance spectrum will become wider with the increase of $\Delta \theta$. For Fano resonance with different degrees of asymmetry, the electric field is shown in figure 6. When $\Delta \theta = 10^\circ$, the dipole mode is displayed at 4.92 THz; therefore, there is more or less no resonance. When $\Delta \theta$ increases to 20$^\circ$, the opposite type of charge accumulates in the gap; the upper and lower rings generate a reverse parallel current, showing a magnetic dipole mode; and the Fano resonance appears. If $\Delta \theta$ increases further, the charge density of the gap increases further, and the corresponding Fano resonance peak increases.

In addition, we also observed the results by changing the polarization angle. Figure 7(a) is the result of our simulation. Since our structure is asymmetric, the polarization angle increases from 0$^\circ$ to 45$^\circ$ and the resonance result changes obviously. Figure 7(b) is the result obtained by theoretical fitting, which is basically consistent with the simulation curve in figure 7(a), indicating that the resonator we designed is of practical significance.

### 4. Sensing performance

To study the sensitivity of the structure, we assume that the DSFs layer is covered with an additional layer of the object to be tested. First, the effect of the thickness of the analyte on the Fano and quadrupole resonance is analyzed. We set the Fermi level and refractive index at 90 meV and 1.43 (Poly tetra fluoroethylene (PTFE)), respectively, and the thickness of the object to increases from 60 to 240 nm. As shown in figure 8(a), when the electric polarization is perpendicular to the two gaps, the thickness of the object increases, the Fano resonance

![Figure 5](image-url-for-figure-5) **Figure 5.** For different asymmetry: (a) simulation curves and (b) fitting curves.

![Figure 6](image-url-for-figure-6) **Figure 6.** The distribution of the electric field with Fano resonance based on the increasing asymmetric degree from 10$^\circ$ to 40$^\circ$.

| $\Delta \theta$ | $\kappa$ | $\gamma_1$ | $\gamma_2$ |
|---------------|---------|------------|------------|
| 10$^\circ$    | 0.073   | 0.721      | 2.376      |
| 20$^\circ$    | 0.187   | 0.685      | 2.152      |
| 30$^\circ$    | 0.742   | 0.645      | 1.938      |
| 40$^\circ$    | 1.341   | 0.650      | 1.765      |

Table 1. Fitted parameters for different $\Delta \theta$. 

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shows a monotonous red-shift because of the increase in the effective dielectric constant of the top layer. The frequency shift is 0.13 THz. Similarly, when the electric polarization is perpendicular to the two gaps, as shown in figure 8(b), the quadrupole resonance also shows a red shift with increasing thickness, and the frequency shift is 0.21 THz.

Next, we study the resonance transmission spectrum of different analytes with different refractive indexes, setting the thickness to 60 nm and the Fermi level to 90 meV, respectively. The results are shown in figures 9(a) and (b), as the refractive index of the analyte increases, both the frequencies of the Fano resonance and the quadrupole resonance show red shift. The following refractive indexes represent important technical indicators for the THz sensing technology; Chemicals—PTFE ($n = 1.43$), Hexogen (RDX ($n = 1.66$)), and TNT ($n = 1.76$); biological materials—air-dried Herring DNA ($n \approx 1.65$) and Ovalbumin ($n \approx 1.15$) [34].

To quantitatively describe the sensitivity of the designed structure, we calculate and plot the resonant frequency shift as a function of the refractive index of the analyte for a fixed thickness of 60 nm. As shown in figure 10(a), the frequency shift of the Fano and quadrupole resonance increases linearly with the increase in the refractive index of the analyte. The slope of the linear shift of quadrupole resonance is greater than the Fano resonance, which signifies that the quadrupole resonance has high frequency sensitivity. Defining the frequency sensitivity as $df/dn$, the frequency sensitivity values of the Fano resonance and the quadrupole resonance are 0.2 THz/RIU and 0.38 THz/RIU, respectively. Then, we calculate the influence of the thickness of different analytes on the sensitivity. Figure 10(b) shows the quadratic fitting curve. It can be seen that as the thickness of the analyte increases, the frequency sensitivity becomes larger. The frequency sensitivity values of the Fano resonance and the quadrupole resonance reach 0.6 THz/RIU and 0.933 THz/RIU, respectively, when the thickness of the analyte is 240 nm. In addition, the rate of sensitivity tends to saturate when the thickness is $>240$ nm.

Finally, to analyze the tunable property of the asymmetric Dirac semimetal split ring structure, we simulated the amplitude transmission spectra of DSFs at different Fermi levels. The simulated results are shown in
Figure 9. (a) Fano resonance and (b) quadrupole resonance with analytes of different refractive indexes. The Fermi level is 90 meV, and the thickness of the analyte is 60 nm.

Figure 10. (a) Resonant frequency shift of the Fano and quadrupole resonance varies with the refractive index. The thickness of the analyte to be tested is 60 nm; (b) relationship between thickness of analyte and frequency sensitivity of the Fano and quadrupole resonance.

Figure 11. (a) The amplitude transmission spectrum of different Fermi energy levels when the electric polarization is perpendicular to the gap. (b) The amplitude transmission spectrum of different Fermi energy levels when the electric polarization is parallel to the gap.
figures 11 (a) and (b); as the Fermi level increases from 90 to 100 meV, the frequencies of the Fano and quadrupole resonance show blue-shift. The frequency peaks of the Fano and quadrupole resonance can be adjusted within the range of 4.92–5.33 THz and 9.63–10.72 THz, respectively. The corresponding modulation depth of the frequency is 7.69% for Fano resonance and 10.17% for quadrupole resonance.

5. Conclusion

We have prove that the ASR structure based on Dirac semimetals offers Fano resonance with a high Q factor in the THz band, and the Q factor can reach 20.19. An amplitude modulation of 27.19% has been achieved by increasing $\Delta \theta$ of the asymmetric split ring from $10^\circ$ to $40^\circ$. Meanwhile, our full-wave electromagnetic simulations show that the frequency sensitivity values of Fano and quadrupole resonance are as high as 0.6 THz/RIU and 0.933 THz/RIU. In addition, the sensing range can be adjusted by altering the Fermi levels of Dirac semimetals. The results contribute to the detection of biological and chemical molecules in the THz range, and the design of ultrasensitive sensors.

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