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Tunable terahertz circular dichroism based on graphene-metal hybrid metasurface

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Abstract: *Chiral metasurface shows a strong ability to control circularly polarized electromagnetic waves, and the introduction of dynamic-manipulation will further expand the application potential for chiral meta-devices. In this paper, we propose a new scheme to realize tunable chiral terahertz devices. By introducing patterned monolayer graphene into the reflective chiral metal meta-atoms, the chiral terahertz response of the metasurface is efficiently and dynamically adjusted, and its reflective circular dichroism value gradually changes from -0.7 to -0.2. In addition, the change of the incident angle may cause the symbol inversion of circular dichroism and change it from single-band to multi-band. We analyze the physical mechanism of tunable chiral response caused by Fermi level of graphene and the principle of the dynamic change of reflection circular dichroism. The proposal of this scheme provides a new idea for the dynamic tuning of chiral metasurfaces and promotes the development of tunable terahertz meta-devices.*

Keywords: *terahertz; metasurface; graphene; circular dichroism*

1. Introduction

The chirality of objects exists widely in nature, such as double helix DNA molecules, human hands, and some galaxies in the universe. The electric field oscillation trajectory of circularly polarized light shows a three-dimensional spiral structure in the propagation direction, which is also chiral. Interestingly, the chirality of light interacts with the chiral optical media, which is called chiral optical response. This phenomenon can be explained intuitively that chiral optical media show different refractive indexes for two kinds of circularly polarized light, and their real or imaginary parts correspond to circular birefringence and circular dichroism, respectively. The circular dichroism of the substance can be used to distinguish chiral isomers, and has been widely used in biomedicine, chemical industry and other fields[1]. However, the circular dichroism of natural materials is mainly caused by electron level transitions (electronic circular dichroism, ECD) or molecular vibrations (vibrating circular dichroism, VCD), which are very weak on the spectrum and therefore require higher measurement accuracy [2,3]. Metasurface is an artificially designed two-dimensional wavelength meta-atomic array, which has unique advantages in wavefront regulation and near field enhancement [4-6]. Chiral or non-chiral metasurfaces may cause strong interactions between chiral light fields and chiral substances, so they are used to enhance the circular dichroism of chiral molecules. In addition, the light field control function of chiral metasurface itself has also attracted much attention, such as chiral wavefront control, efficient spin selective absorption, polarization multiplexing phase control and so on.

The tunable metasurface can dynamically control the response of the incident electromagnetic wave, such as amplitude, polarization, phase, wavefront and even spin and orbital angular momentum, which is expected to be used in communication, imaging, information processing and so on [6]. There are many ways to realize tunable metasurface, including light, electricity, heat, force, micromachinery and so on. In the terahertz band, because it has some characteristics of both optics and microwave, the metasurface is especially suitable to be used as a tunable research object, and there are various modulation modes.

Graphene shows good conductivity and flexible properties, through electro-doping can produce a large number of carriers, its Fermi level can be dynamically adjusted over a wide range, so it is one of the effective realization of terahertz tunable metasurfaces [9]. On the other hand, the circular dichroism of terahertz wave is also one of the important phenomena of chiral metamaterials, because the terahertz frequency is closely related to the weak rotation and vibration of macromolecules, so it has a wide application prospect in biomedical and other fields. Therefore, the regulation of terahertz circular dichroism is also particularly important. At present, the dynamic control of terahertz CD includes optically pumped silicon, phase change materials and so on. However, the modulation depth of these controls is limited [10]. Graphene-based terahertz CD modulation appears to be more effective, but there is little research in this area.

In this paper, we propose a terahertz CD dynamic control scheme based on metal-graphene hybrid metasurface. Hollow graphene is introduced into the dielectric isolation layer of double-layer C-shaped metal open-ring reflective chiral meta-atoms, and the Fermi level of graphene is changed by electro-doping, and then the terahertz circular dichroism of the device is changed. We have systematically studied the tunable circularly polarized reflection characteristics of the metasurface. The calculation results show that this structure has a great modulation depth and can realize the perfect switching from the chiral structure to the ordinary mirror state of the metasurface.

2. Model and theoretical analysis

In the absence of an external bias magnetic field, the conductive properties of graphene in the band below the infrared frequency are mainly generated by in-band transitions, and its equivalent conductivity can be calculated from the simplified Kubo formula [7] :

$$\sigma_g \approx \sigma_{\mathrm{intra}} = i\frac{e^2 K_B T}{\pi h^2(\omega + i\Gamma)}\left[\frac{E_F}{K_B T} + 2\ln\left(\exp\left(-\frac{E_F}{K_B T}\right) + 1\right)\right] \tag{1}$$

E_F is the Fermi level of graphene, T is the Kelvin temperature, and the carrier scattering rate (the inverse of the relaxation time τ) is the Γ. For weakly doped graphene, the formula can be expressed in Drude form if conditions $|E_F| >> K_B T$ and $|EF| >> K_B T$ are satisfied.

$$\sigma_g = \frac{iD}{\pi(\omega + i\Gamma)} = \frac{ie^2 E_F}{\pi h^2(\omega + i\Gamma)} \tag{2}$$

where D is the Drude mass and the Fermi level is a function of the carrier concentration:

$$|E_F| = hV_F(\pi|n|)^{1/2} \tag{3}$$

It can be seen that graphene Fermi level can be adjusted by doping, chemical surface modification, applied voltage, magnetic field and other ways.

In addition, according to Jones matrix theory, the incident and reflected waves of anisotropic metasurface elements can be related by transmission coefficient matrix.

$$\begin{pmatrix} \mathrm{E}_x^r \\ \mathrm{E}_y^r \end{pmatrix} = \begin{pmatrix} r_{xx} & r_{xy} \\ r_{yx} & r_{yy} \end{pmatrix}\begin{pmatrix} \mathrm{E}_x^i \\ \mathrm{E}_y^i \end{pmatrix} \tag{4}$$

According to the relationship between the linearly polarization wave and the circular polarization wave, the circular polarization reflection coefficient of the reflective wave can be obtained:

$$\begin{pmatrix} r_{++} & r_{+-} \\ r_{-+} & r_{--} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} r_{xx} + r_{yy} + i(r_{xy} - r_{yx}) & r_{xx} - r_{yy} - i(r_{xy} + r_{yx}) \\ r_{xx} - r_{yy} + i(r_{xy} + r_{yx}) & r_{xx} + r_{yy} - i(r_{xy} - r_{yx}) \end{pmatrix} \tag{5}$$

For reflective chiral metasurface, R+- is equal to R-+, while R++ is not equal to R--.

3. Results and discussion

The metal-graphene chiral metasurface proposed by us is shown in **FIG. 1 (a)**, Take the function in the figure for example, its in-plane mirror structure will have the opposite function. When a left-handed circularly polarized (LCP) terahertz wave is incident, most of the wave will be converted to a right-circularly polarized (RCP) reflected wave, while when a right-circularly polarized wave is incident, a significant portion of the energy will be absorbed. For the sake of intuition, the part of the figure where the incident angle is not active is not shown.

To achieve the above functions, we designed a chiral metasurface unit as shown in **FIG. 1 (b)**. Based on the design principles of chiral metasurface, we need to break both the mirror symmetry and the nfold(n≥2) rotation symmetry of the structure, Graphene is also needed for dynamic adjustment. Thus, the meta-atom consists of a metal backplane, two S-shaped resonators, a hollow monolayer of graphene, and an insulating material, with two S-shaped units having an angle. Meta-atomic period P=180 microns, the height of the two resonators and graphene from bottom to top is H_1=6 μm, H_2=20 μm, H_3=50 μm. The width of the metal strip is W μm, and the hollow radius of graphene is R=85 μm; We simulated the unit using the frequency domain solver of the CST Microwave Studio, X and Y directions are set as unit cell boundary conditions, and z directions are set as open boundaries. During the simulation, the dielectric constant of polyimide was set as 3.5 and the tangent of loss angle was 0.0027. During the simulation, the chiral response of the metasurface is adjusted by setting the graphene Fermi level to different values.

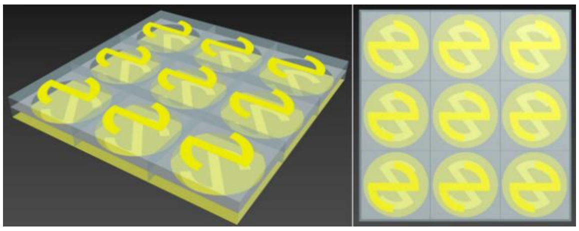
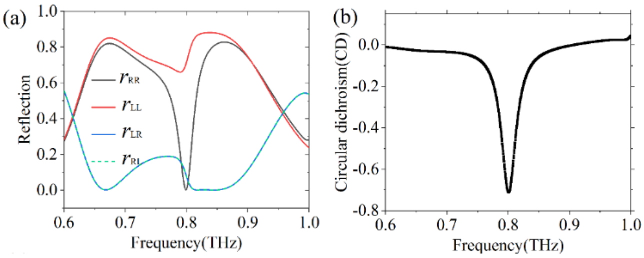


Figure 1: Schematic diagram of a chiral metasurface.

First, we calculate the original chiral response, as shown in **FIG. 2**. We set the Fermi level of graphene to 0.01eV, we obtain significant absorption differences in the circularly polarized reflectance spectra. As can be seen from **FIG. 2 (a)**, For the shape of the structure that we're emulating, the RCP incident wave is absorbed efficiently at 0.8 THz, whereas LCP waves are absorbed very weak, most of the energy is reflected. In addition, the two cross polarization components are small, values near 0.8 THz approach 0. Based on these results, we calculated the circular dichroism at this time, as shown in **FIG. 2 (b)**, the difference in peak absorption rate is about 0.7. The reflectivity of each polarization component is R=r^2. The absorption difference can be calculated by

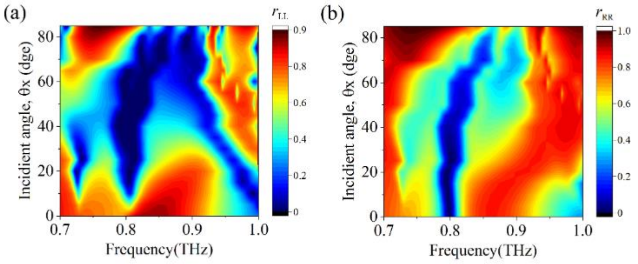
$$R_{CD}=A_R-A_L=R_{LR}+R_{RR}-R_{RL}-R_{LL} \qquad (6)$$



(a) Reflection coefficient of circular polarization; (b) Circular dichroism of reflection.

Figure 2: Reflection spectra of chiral metasurface at Fermi level of 0.01eV.

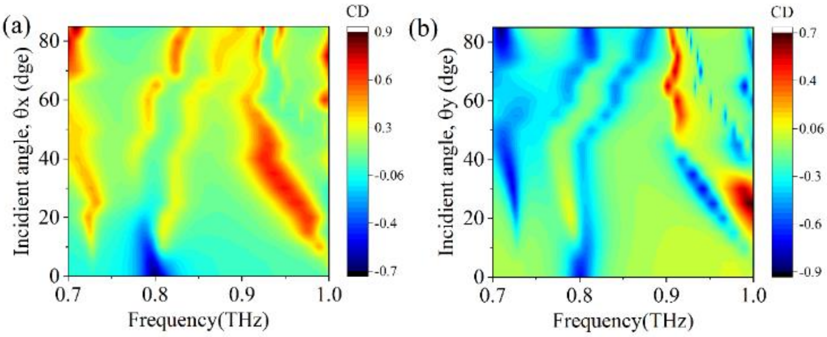
Next, we investigate the sensitivity of the chirality response to the incident angle. Without loss of generality, we change the incident angle of the incident wave in plane xoz, and calculate the reflection coefficients r_{LL} and r_{RR}, as shown in **FIG. 3**. Obviously, due to the complexity of structural symmetry, reflection coefficient is sensitive to incident angle. When the angle is greater than about 10 degrees, the reflection coefficient of LCP incident wave decreases sharply and keeps a very small value. For the RCP incident wave, it keeps a small reflection coefficient at 0.8THz, but only shows a small frequency shift.



(a) rLL at different incidence angles; (b) rRRat different incidence angles

Figure 3: Influence law of incident Angle on reflection coefficient.

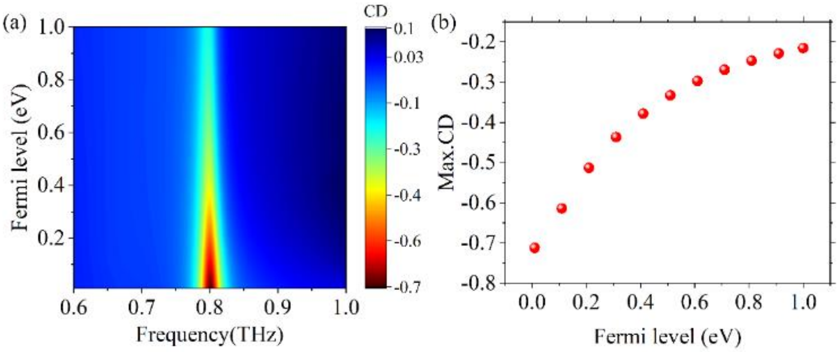
In addition, in order to show the effect of incident angle on the circular dichroism of reflection more directly, we also calculate the reflection circular dichroism under different incident angle. **FIG. 4** shows the reflection circular dichroism obtained by changing incident angles in xoz and yoz planes. It can be found that around 0.8 THz, the reflection circular dichroism is sensitive to the incidence angle, This is consistent with the variation rule of reflection coefficient in **FIG. 3**. It is worth noting that, with the increase of the incidence angle, there is a large difference in the absorption rate at other frequencies, and the value of circular dichroism changes from negative to positive, which means that the function of the metasurface changes from absorbing RCP waves to absorbing LCP waves, and from single frequency band to multi-frequency band.



(a) CD spectra at different incidence angles θx; (b) CD spectra at different incidence angles θy.

Figure 4: Influence of incident Angle on CD.

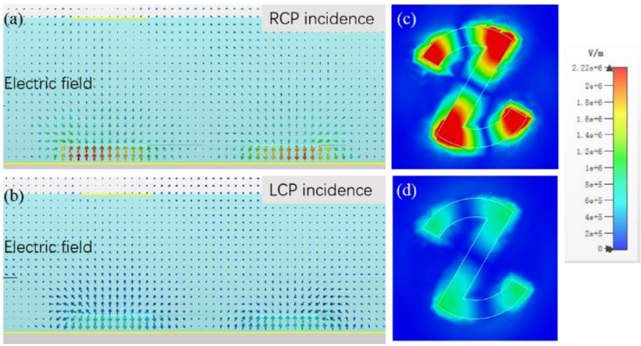
Here we study dynamically tunable chiral responses based on graphene. As already mentioned, the Fermi levels of graphene can be adjusted by bias voltage. We designed a single layer of graphene as a circular hollow structure to reduce the absorption of THz waves by graphene, and placed it between two metal resonators in order to change the chiral response more easily, because the chirality response is mainly caused by the electromagnetic coupling between the resonators. Adjusting the Fermi energy levels of graphene will effectively change their electromagnetic coupling, thus changing the reflective response of the entire device. We gradually increased the Fermi level of graphene from 0.01eV to 1eV, and calculated the reflection circular dichroism under vertical incidence, as shown in **FIG. 5 (a)**. As expected, the change in graphene conductivity effectively changes the chirality response of the metasurface, and the peak frequency of CD is almost unchanged. In order to display the change of CD more intuitively, the peak values of circular dichroism at each Fermi level are given in **FIG. 5 (b).** It can be seen that the peak value of CD changes gradually from -0.7 to -0.2, showing a great dynamic adjustment range and linearity.



(a) CD spectra at different Fermi energy levels; (b) Peak values of CD at different Fermi levels;

Figure 5: Effect of graphene Fermi level on circular dichroism.

Finally, in order to explain the physical mechanism of chiral absorption of our proposed structure, we give the local electric field distribution diagram in the superatom under RCP and LCP wave incidence in **Figs. 6(a)** and **6(b)** show the vector distribution of electric field in xoz section. Obviously, all this in-plane electric field is concentrated between the resonator below and the metal backplane when the RCP wave is incident. However, there is no obvious local electric field enhancement when LCP wave is incident. **Figs. 6(c)** and **6(d)** show the electric field intensity distribution in the XOy section near the bottom S-shaped resonator. It can be found that the distribution of electric field intensity is consistent with the vector distribution in the figure on the left, further confirming the direct cause of the chirality response of the meta-atom.



(a) Electric field distribution in xoz plane(vector); (b) Electric field intensity distribution in xoy plane;

Figure 6: Physical mechanism of the chirality influence;

4. Conclusion

In conclusion, we design a tunable terahertz chiral metasurface based on a graphene-metal hybrid structure. The effect of incident angle on the reflection coefficient and circular dichroism was studied. By introducing a monolayer graphene between two metal resonators and changing the Fermi levels of it by applying a bias voltage, we have a wide range of tuned circular dichroism, its peak value can vary from -0.7 to -0.2. The effect of incident angle on circular dichroism is also studied. The results show that the change of incident angle causes the peak value of reflection circular dichroism to change from negative to positive and from single operating band to multi-frequency band, which provides a new degree of freedom for the regulation of chirality response. The proposed scheme provides a new reference for the design of chiral metasurface.

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