Tunable chiral responses in mechanically reconfigurable three-dimensional metamaterials

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Keywords: selective transmission, circular dichroism, polarization conversion, mechanical tunability

Supplementary material for this article is available online

Abstract

The active manipulation of polarization state is of fundamental importance to functional devices integrated in modern terahertz (THz) systems. The emerging chiral metamaterials (MMs) provide enormous possibilities to control the polarization state of incident THz wave, however, existing MMs with strong chirality are normally insufficient to modulate the circular dichroism (CD). Here, we have proposed a conceptual 3D mechanically reconfigurable chiral MM that is capable of tailoring the right circular polarization transmission and linear-to-circular polarization conversion. The 3D MM morphology can be reproducibly controlled by alternating the pre-strain on the elastic substrate, which allows to provide a flexible route to reconfigure the structural chirality and modulate the chiral response. Additionally, CD spectra exhibit high sensitivity to the rotation angle of MM component. The mechanically tunable chiral MM with high flexibility will build up an efficient approach for the CD enhancement and modulation and paves a novel avenue toward the reconfigurable design principle of flexible functional THz devices.

1. Introduction

Recent advances in the terahertz (THz) science and technology have promoted considerable varieties of applications such as wireless communication, \([1]\) imaging, \([2]\) chemical detection \([3]\) and biosensing \([4]\) due to THz intrinsic physical properties including large bandwidth, short wavelength and fingerprint spectrum. Chirality, referring to the configuration that is lack of mirror symmetry and thus cannot superimpose its mirror structure, is a ubiquitous phenomenon ranging from organic molecules such as proteins and DNAs to the shape of galaxies in the nature. Due to the structural chirality including left-handedness and right-handedness, the circularly polarized waves including left circular polarization (LCP) and right circular polarization (RCP) propagate with diverse absorptions, defined as circular dichroism (CD). Additionally, the response of linearly polarized wave toward chiral structure often exhibits the rotation of polarization state that results from distinct refractive indexes for LCP and RCP waves \([5]\). Despite the practical prospects in the polarization modulation and conversion, \([6, 7]\) the chirality in natural materials is normally too weak to sufficiently meet the engineering requirement in the photoelectric field \([8]\). Therefore, it is imperative to artificially design chiral micro-scale structures integrated in modern photonic devices to strongly enhance the structural chirality and efficiently modulate the spin state or polarization direction of incident THz wave.

Metamaterial (MM), consisting of periodically arranged subwavelength constituents, provides large degree of freedom for manipulating the amplitude, \([9]\) phase \([10]\) and polarization \([11]\) of the THz wave and greatly facilitates the performance of conventional photonic devices. Relying on the symmetry breaking of unit morphologies, MMs can greatly promote structural chirality to achieve distinct

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transmission or absorption under the LCP and RCP excitation. The chiral MMs developed in recent years exhibit several orders of magnitude larger CD than that of natural media, which makes them extremely suitable in negative refractive index materials, [12, 13] circular polarization detector, [14, 15] chiral imaging [16, 17] and polarization conversion. [18, 19] Owing to non-uniform geometries, 3D MMs dominate the large family of chiral MMs on modulating the polarization state of incident wave including multi-layer stackings, [20, 21] helical structures [22–24] and spatial chiral networks [25, 26] etc. However, non-symmetric complex 3D structures along the normal direction bring huge challenges in the fabrication procedure. For example, Kaschke et al. have proposed helical MMs by following a series of experimental procedures including direct laser writing of helical voids, electrochemical gold deposition and the removal of residual photoresist in the oxygen plasma. [27] On the other hand, prevalent chiral MMs ordinarily have unalterable and unreconfigurable morphologies which do not allow their dynamic modulation on the chiral electromagnetic (EM) response. It can be seen that the tedious fabrication procedure as well as the non-tailorable reconfiguration will ultimately hinder the emerging development of 3D MMs-based chiral devices.

Mechanically tunable MMs by strain induced in-plane deformation have been growing unprecedentedly to modulate the EM transmission and absorption spectra at THz frequencies [28, 29]. For example, Fan et al. [30] and Xu et al. [31] have proposed deformable metasurfaces by integrating the periodically arranged subwavelength structures with the flexible substrate and successfully manipulated the resonant frequency and transmission amplitude through the change of the configuration and the periodicity of unit cells. However, these mechanically tailored MMs are mostly dependent on the 2D deformation and thus are inapplicable to break the symmetry in the vertical dimension to enhance the chirality. Recently, researchers have proposed to take full advantage of residual stress in the pre-stretched flexible substrate to fabricate a number of fascinating 3D microstructures including scorpion, [32] rodent, [33] and flower. [34] These mechanical assembled structures can be freely manipulated by the pre-strain induced symmetry breaking along the normal dimension and may shed light on the unconventional design and fabrication guideline to achieve reconfigurable chiral MMs.

In this work, we propose a novel type of mechanically reconfigurable chiral MM consisting of two split-ring resonators (SRRs) in the unit cell that are transversely arranged with rotational symmetry. The out-of-plane 3D MM with rotational symmetry induced by the release of strain energy stored in the stretched planar substrate shows its controllability in the enhancement of structural chirality. The dynamic effect of mechanical strain on the spin-selective transmission upon LCP and RCP incidence will be thoroughly investigated by different pre-strains of the substrate. Furthermore, the relative angle between

Figure 1. Geometrical schematics and formation principle of the mechanically reconfigurable MM. (a) The geometrical parameters of the planar precursor consisting of four-layer gold/PEN/PI/PI structure. (b) The schematic illustration of mechanically reconfigurable MM. The dynamic deformation process can be seen in multimedia view 1. (c) The displacement distribution of the buckled unit cell with the pre-strain $\varepsilon_{\text{pre}}$ as 7.5%, 15%, 30%, 45%,
Figure 2. The transmission and CD spectra for planar and deformable MMs. (a)–(e) The transmission spectra of the MMs induced by the pre-strain $\varepsilon_{\text{pre}} = 0, 7.5\%, 15\%, 30\%, 45\%$ upon LCP and RCP incidence. Insets: top-view of the MMs in different deformation stages. (f) The CD spectra of MMs with different pre-strain.

two SRR gaps can also manipulate the chiral response. Our proposed method could provide a mechanical approach toward tunable chiral MMs and build up a brand-new platform for exploring reconfigurable flexible THz devices.

2. Model

The proposed mechanically reconfigurable MM precursor is schematically shown in figure 1(a). The MM unit cell is composed of four-layered components including SRR pair closely attached on two independent stiff square plates, a passively out-of-plane deformable supporting layer and an actively in-plane deformable substrate. Two 0.5 $\mu$m-thick gold SRRs are patterned with rotational symmetry to disintegrate the mirror symmetry in the horizontal plane. The geometric and electrical parameters of SRRs are given by the periodicity $P_x = P_y = 80$ $\mu$m, the inner radius $r_1 = 12$ $\mu$m, the outer radius $r_2 = 16$ $\mu$m, the gap $g = 4$ $\mu$m and the electric conductivity $\sigma = 4.561 \times 10^7$ Sm$^{-1}$, respectively. The PEN material with the relative permittivity as 2.56 and the loss tangent as 0.003 [36] is taken into account for the 1.5 $\mu$m-thick plates to balance its low dielectric loss and high elastic modulus, and geometrical parameters of the plates are optimized as the width $a = 38$ $\mu$m and the height $b = 40$ $\mu$m. The flexible 0.5 $\mu$m-thick passive layer and 30 $\mu$m-thick active substrate are made of polyimide (PI) with the relative permittivity as 3.24 and the loss tangent as 0.031. [36] To investigate the chiral responses of proposed structures upon LCP and RCP
incidence, the transmission coefficients and current density are numerically simulated by utilizing CST microwave studio.

Figure 1(b) schematically shows the mechanically reconfigurable mechanism of the proposed MM. Initially, the free flexible substrate is uniaxially stretched to a pre-strained state with \( \varepsilon_{\text{pre}} = \Delta L / L = 45\% \) where \( \Delta L \) is the change in length and \( L \) is the original length of the substrate. Then the red region of the passive layer with the width \( d = 10 \mu m \) is tethered on the pre-stretched substrate, and finally the in-plane SRRs deform into the out-of-plane configuration when the substrate restores to its initial length. The mechanical properties of all materials are modeled by the linear elastic relation with the elastic modulus \( (E) \) and Poisson’s ratio \( (\nu) \) given by \( E_{\text{gold}} = 78 \) GPa, \( \nu_{\text{gold}} = 0.44, E_{\text{PI}} = 2.5 \) GPa, \( \nu_{\text{PI}} = 0.34, E_{\text{PEN}} = 5.2 \) GPa and \( \nu_{\text{PEN}} = 0.37 \), respectively. [37] The square plate with large elastic modulus can provide the rigid motion of SRRs and prohibit their deformation during the buckling process. The whole self-assembled procedure driven by the release of pre-strain of the active substrate results in the large degree bending of the passive layer. All mechanical simulations are performed by Abaqus software. For the bonding constraints, the structure with large elastic modulus possesses sparse mesh to guarantee the computational accuracy.

To testify the geometrical modulation mechanism of proposed MM shown in figures 1(b) and (c) shows the morphologies of unit cells as well as their displacement distribution under the pre-strain as \( \varepsilon_{\text{pre}} = 7.5\%, 15\%, 30\%, 45\% \) on the substrate. It can be evidently observed that the pre-strain increment facilitates the bending displacement of the central region of passive layer and shortens the center-to-center space distance between SRR pair, which might trigger some intriguing coupling effects under the THz incidence.

3. Results and discussion

In order to evaluate the chiral response of mechanically reconfigurable MMs, distinct 3D unit cells are investigated upon LCP and RCP incidence. As a reference shown in figure 2(a), the transmission coefficient of 2D planar MM exhibits identical profile for opposite spin states of THz wave. In spite of the symmetry breaking in the horizontal plane, 2D structure scarcely possesses requisite asymmetry in the normal direction to the substrate, which results in trivial structural chirality and chiral response. By contrast, the transformation of 2D MM into 3D configuration promotes the symmetry breaking along the normal direction. As shown in figures 2(b)–(e), 3D buckled MMs under the pre-strain \( \varepsilon_{\text{pre}} = 7.5\%, 15\%, 30\%, 45\% \) applied on the flexible substrate can distinguish the spin state of circularly polarized wave and the transmission spectra for LCP and RCP incidence. When \( \varepsilon_{\text{pre}} \) increases from 0 to 45\%, the transmission profiles for LCP and RCP are remarkably separated with opposite deep valley and high crest, respectively. Take figure 2(e) as an example, the transmission amplitude of the LCP incidence is greatly suppressed low to 0.22 at the resonant frequency of 1.304 THz, while the RCP wave can propagate with the maximum amplitude of 0.94 around 1.286 THz. It is worthwhile to clarify that such deformable MMs can provide high transmission for RCP incidence but block the transmission of the opposite one. In turn, the favorable transmission for LCP wave can also be promoted by exchanging the arrangement of SRR pair, which demonstrates its spin selectivity by 3D mechanical deformation. Additionally, the opposite evolution in the transmission amplitude induces high contrast of LCP and RCP waves and thereby enhances the CD amplitude of 0.94 around 1.286 THz. Due to the flexibility of the 3D buckled unit cell, the CD can be reversibly tuned through the mechanical stretching of the 3D deformed device. By taking the 3D deformed MM with \( \varepsilon_{\text{pre}} = 45\% \) as example, it can be conversely stretched back to the planar state and the periodicity along the \( x \)-direction continuously increases from 80 \( \mu m \) to 116 \( \mu m \). During the stretching process, the maximum CD reduces from 0.82 to 0 and the resonant frequency for LCP incidence shifts from 1.30 THz to 1.16 THz (figure S1) (https://stacks.iop.org/NJP/23/053001/mmedia). Overall, the performance of the reconfigurable MM on the tunable chiral response can be dynamically modulated by stretching or releasing the flexible substrate.

Recently, advances in Kirigami-based reconfigurable structures also have presented applications in the mechanically tunable chiral MM [38], which are designed to be ultra-thin for easy folding and operate at GHz frequencies. In this MM, a unit cell consisting of four SRRs is required to realize the enhancement of the symmetry breaking and CD. In contrast, our proposed meta-atom with two SRRs is simplified and the CD value can reach 0.82 when the SRR pair is transformed from a planar state to an arch shape. Moreover, the Kirigami structure can only fold along a tailored direction dependent on the cutting path, but the 3D assemble method enables uniaxial and biaxial deformation of structures [39], which may provide more potentials for MM design.

The spin-selective transmission in the deformable MM can be further extended to the conversion of linear-to-circular polarization. When a linear polarized wave via the superposition of LCP and RCP wave
with identical amplitude impinging on the proposed spin-selective MM, the RCP component can transmit efficiently while the LCP component is blocked and hence the linear polarized wave is converted into the RCP wave. In order to verify the linear-to-circular conversion process, figures 3(a) and (b) depicts the amplitude and phase difference of $x$- ($t_{xx}$) and $y$-direction ($t_{yx}$) transmission upon $x$-polarization incidence. It can be observed that the transmission amplitude of $t_{xx}$ and $t_{yx}$ intersects at 1.292 THz and the phase has $90^\circ$ difference at 1.294 THz. In other words, the transmitted wave exhibits nearly circular polarization state.
from 1.292 THz to 1.294 THz. Consequently, the proposed MM can be utilized to achieve the linear to LCP conversion by exchanging the arrangement of SRR pair.

To illustrate the underlying physical mechanism of the tailored transmission, the magnetic flow and surface current at the resonance are systematically analyzed. Figure 4(a) shows the magnetic field along the z-direction in the planar MM at the resonance, which indicates that SRR pair localizes the magnetic field with opposite direction and generates two opposite magnetic dipoles (MDs) \( m_1 \) and \( m_2 \) inside the SRRs. The anti-parallel oscillation of two MDs excites the resonance at 1.12 THz upon LCP/RCP incidence to the planar MM. For the deformed MM with \( \varepsilon_{\text{pre}} = 45\% \) upon the LCP incidence shown in figure 4(b), the magnetic flow in the x–z plane is featured with an anti-clockwise loop. As shown in figure 4(c), there emerges loop current along SRR pair due to the strong coupling between LCP incident wave and SRR pair, which gives rise to two MDs with a relative angle and agrees well with magnetic flow in figure 4(b). On the other side, the current flow on the SRRs induces the concentration of positive and negative charges or electric dipoles (EDs) on two sides of the gaps. In the case of RCP incidence in figure 4(d), similar loop...
current can also be excited but with extremely weak intensity, which suggest that the MM possesses weak interaction with the incident RCP wave. All observations from magnetic flow and surface current clearly reflect the resonant intensity between opposite spin states and illustrate the deformation-induced chiral responses. To quantitatively analyze the contribution of different dipoles on the resonance, the radiative power of different multipoles in the deformable MM is calculated for LCP and RCP incidence by the general multipole scattering theory as [40, 41]

\[
I = \frac{2\omega^4}{3c^4} |P|^2 + \frac{2\omega^4}{3c^4} |M|^2 + \frac{2\omega^6}{3c^6} |T|^2 + \frac{\omega^6}{3c^6} \sum |Q_{\alpha\beta}|^2 + \frac{\omega^6}{4c^6} \sum |M_{\alpha\beta}|^2 (\alpha, \beta = x, y, z),
\]

where \( P, M, T, Q_{\alpha\beta} \) and \( M_{\alpha\beta} \) represent the ED, MD, toroidal dipole, electric quadrupole and magnetic quadrupole, \( \omega \) is the angular frequency and \( c \) is light speed in the vacuum. Figures 4(e) and (f) show the scattering power for multipole moments in the deformed MM (\( \varepsilon_{pre} = 45\% \)) for LCP and RCP incidence, respectively. From figure S2, the \( x \)-component of ED moment \( (P_x) \) and \( x \)-/y-components of MD moment \( (M_x \text{ and } M_y) \) have larger dispersion than that of other components, and thereby the scattering power of these dominant components are considered here. For the LCP THz wave impinging on the deformable MM, the \( x \)-component of ED moment and \( x \)-/y-components of MD moment dominate the dispersion and the maximum scattering power locates at the resonant frequency. Similar observations can be found for RCP incidence but the scattering power corresponding to ED and MD moments has low magnitude. The total scattering power for LCP incidence is almost one order of magnitude larger than that for RCP incidence, which agrees well with the higher resonant intensity for LCP than that for RCP in the transmission spectra in figure 2(e).

Relying on the physical mechanism that the resonance originates from the excitation of electric and MDs, the mechanical modulation of CD spectrum in the proposed MM can be testified by the multipole analysis under various applied pre-strain \( \varepsilon_{pre} \). As shown in figure S3, when \( \varepsilon_{pre} \) applied in the reconfigurable MMs increases, the LCP incident wave strongly enhances the excitation of MDs while the scattering spectra for EDs fluctuate with a minor amplitude, which results in the strong resonant intensity (blue curves) in the figures 2(a)–(e). For RCP wave impinging on the deformable MMs, the scattering power evolves towards low magnitude compared with the dispersion of planar configuration, which verifies the high transmission (red curves) in figures 2(b)–(e). Furthermore, the current density \( |J| \) (insets of figure S3) in different deformable MMs is promoted under LCP incidence and weakened under the RCP incidence, which can also prove the enhanced resonant divergency and agrees well with the multipole analysis.

In analogy with the pre-strain effect on the modulation of CD spectra, the effect of rotation angle with respect to deformed SRR pair is also investigated to unveil its influence on the resonant response for LCP and RCP incidence. As shown in figure 5(a), the left SRR rotates anticlockwise with the angle \( \alpha \) while the right SRR remains unchanged. Figure 5(b) shows the CD spectra for \( \alpha \) from \( 0^\circ \) to \( 180^\circ \). It can be observed that there always exists a high peak in the CD spectra except for the case when SRR pair is symmetrically arranged with \( \alpha = 180^\circ \). When increasing \( \alpha \) from \( 0^\circ \) to \( 110^\circ \), the maximum CD gradually reduces from 0.82 to 0.20 along with the blue-shift of the frequency from 1.30 THz to 1.34 THz. Additionally, when increasing \( \alpha \) to \( 30^\circ \), another peak emerges at the high frequency but with relatively weaker amplitude than that at the low frequency until \( \alpha = 100^\circ \), and it experiences a red-shift over the frequencies. Similar to the deformable MM under \( \alpha = 0^\circ \) as shown in figure 2(e), the transmission spectra upon LCP and RCP incidence shown in figure 5(c) are both split into two resonant valleys for \( \alpha = 90^\circ \). For \( \alpha = 110^\circ \), the peak at the low frequency exhibits low level than that at the high frequency and even disappears when \( \alpha \) exceeds \( 120^\circ \) due to the simultaneous blue- and red-shift of two peaks. Overall, the rotation angle can not only manipulate the amplitude of CD spectra but also alternate the frequency and CD peak.

To better understand the split feature of the transmission spectra, the surface current distributions at two resonant frequencies (\( \omega^- \) and \( \omega^+ \)) are investigated for LCP incidence. As shown in figure 6(a), the left and right SRRs exhibit a clockwise and anti-clockwise current loop at the low resonance \( \omega^- \), respectively, which theoretically equalizes two MDs decomposed into \( m_t \) and \( m_e \) components. However, at the high resonance \( \omega^+ \), both SRRs possess anti-clockwise current loop (figure 6(b)), in other words, \( m_t \) and \( m_e \) are anti-parallel and parallel, respectively. According to the dipole coupling model, [42] the side-by-side and end-to-end alignment of two dipoles can be treated as transverse and longitudinal coupling and thus \( m_t \) and \( m_e \) of MDs exhibit transverse and longitudinal coupling, respectively. Without respect to the transverse or longitudinal coupling, the attraction of two dipoles can decrease the internal stored force and give rise to the decrease of resonant frequency, while the repulsive dipoles can increase the resonant frequency. As shown in figure 6(c), the parallel \( m_t \) (red arrow) are attractive and the anti-parallel ones are repulsive, while the parallel (or anti-parallel) arrangement for \( m_t \) (purple color) leads to a repulsion (or attraction). Therefore, anti-parallel \( m_t \) and parallel \( m_t \) will induce the repulsion of two dipoles to generate a high resonance at \( \omega^+ \). In contrast, the parallel \( m_e \) and anti-parallel \( m_e \) attract reciprocally to each other and
hence a low resonant frequency at $\omega^-$ emerges. Consequently, the transmission spectra can be split by two resonant valleys and finally two peaks appear in the CD spectra.

4. Conclusion

In summary, we have proposed a mechanically reconfigurable chiral MM through the intricate geometrical design of two deformable SRRs and systematically analyze its dynamic modulation on the THz responses. By releasing the flexible pre-stretched substrate, the three-layer gold/PEN/PI structure selectively bonded on the flexible substrate is transformed into an out-of-plane morphology, and simultaneously promotes the symmetry breaking along the vertical dimension. The deformable MM exhibit enhanced structural chirality with tailored transmission for RCP incident wave compared with the identical transmission spectra of planar MM, which builds up an applicable pathway for the spin-selective and linear-to-circular polarization devices. More importantly, the CD spectra can be dramatically modulated by applying different pre-strain on the flexible substrate and the CD peak gradually evolves into the high level with the increment of pre-strain. The relative rotation angle of deformable SRR pair shows another tunable strategy for the chiral response and demonstrates two-peak feature of CD spectra induced by the coupling of dipoles at the range from 30° to 110°. The reconfigurable chiral THz MM not only demonstrates its potential of CD modulation, spin selectivity as well as the polarization conversion but also opens a promising new avenue for mechanically reconfigurable flexible devices at the THz regime.

Acknowledgments

This work was supported by the National Natural Science Foundation of China (Grant No. 51805414), Shenzhen Science and Technology Innovation Commission (Grant No. JCYJ20180306170652664) and Natural Science Foundation of Zhejiang Province (Grant No. LZ19A020002) to Liuyang Zhang.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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