Terahertz Polarization Conversion from Optical Dichroism in a Topological Dirac Semimetal

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Topological Dirac semimetals (TDSM), such as Cd$_3$As$_2$ and Na$_3$Bi, exhibits strong optical dichroism with contrasting dielectric permittivity along different crystal axes. However, such optical dichroism is often overlooked in the study of TDSM-based optoelectronic devices, and whether such optical dichroism can lead to unique functionalities not found under the isotropic approximation remain an open question thus far. Here we show that the optical dichroism in TDSM lead to starkly different terahertz (THz) responses and device performance as compared to the isotropic case. Using finite-difference time-domain simulations of a Cd$_3$As$_2$-based metasurface, we demonstrate that such optical dichroism can lead to an unexpected THz wave polarization conversion even if the metasurface structure remains $C_4$ four-fold rotationally symmetric, a practically useful feature not achievable under the isotropic model of TDSM. Our findings concretely reveal the contrasting spectral response between isotropic and anisotropic media, and shed important light on the capability of anisotropic TDSM in THz applications, leading not just to the more accurate device modelling, but also a new route in realizing THz waves polarization conversion without the need of complex device morphology commonly employed in conventional polarization converters.

Three-dimensional (3D) topological Dirac semimetals (TDSM) represents peculiar 3D analogs of graphene whose electronic band structure around the Fermi level disperses linearly in all three orthogonal crystal directions. Being a 3D bulk material with an additional spatial degree of freedom, TDSM is expected to offer greater device design flexibility not found in the atomically-thin graphene sheet while retaining the exotic physical properties of Dirac material systems. 3D TDSMs, such as Cd$_3$As$_2$ and Na$_3$Bi, has been demonstrated to exhibit myriads of unusual transport and optical properties, such as giant magnetoresistance, exceptionally high electrical mobility, ultrafast relaxation dynamics, nonlinear plasmonics, efficient high-harmonic generation, high-temperature linear quantum magnetoresistance and quantum Hall effect. Leveraging on these unusual physical properties, TDSM has been extensively explored as a promising material for a wide array of solid-state device applications, including photodetector, topological transistor, spintronics, metamaterials thermoelectric converters, and electrical contacts to 2D semiconductor.

TDSM is particularly attractive for nanophotonics applications in the terahertz (THz) frequency regime due to the gapless, and linear energy dispersion that are highly beneficial in generating strong THz optical nonlinearity. Computational studies of novel photonic and optoelectronic devices designs, such as optical switch, absorbers, photodetectors, and polarization converters, have been intensively carried out in recent years. However, it is notwithstanding that most of these computational works are performed based on a simplistic isotropic Dirac semimetal conductivity model where the inherent Dirac band structure anisotropy in realistic TDSM crystals, such as Cd$_3$As$_2$ and Na$_3$Bi, are neglected in which the carrier group velocity along two orthogonal directions can differ by one order of magnitude. The inclusion of Dirac band structure anisotropy appreciably modifies the optical properties of TDSM and dramatically transform TDSM into an anisotropic medium with strong optical dichroism. This aspect immediately leads to the following open questions that urgently need to be addressed: What are the key differences between the simplistic isotropic model and the more realistic anisotropic model of TDSM in the computational design of photonic devices? Does the presence of optical dichroism in TDSM improve or degrade the performance of TDSM-based photonic devices? More importantly, can optical dichroism in TDSM be employed to generate unique functionalities not found in the isotropic counterpart?

In this work, we address the above questions by performing a proof-of-concept device simulations of Cd$_3$As$_2$-based TDSM metasurface by explicitly taking into account the optical anisotropy of Cd$_3$As$_2$ crystal. We demonstrate that the far-field transmission spectra and the near-field electric field distributions (EFDs) are drastically different between the isotropic and the anisotropic TDSM model. Intriguingly, under the more realistic anisotropic TDSM model, a highly-symmetric $C_4$ patterns can readily generate THz wave polarization conversion — a peculiar behavior not achievable under the simplistic isotropic materials. These findings reveal a viable route to achieve efficient polarization conversion.

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of THz waves with simple symmetric structures by harnessing the inherent optical dichroism of TDSM, thus circumventing the need of fabricating complex chiral structures or supercells composed of multiple sub-layers and subunits.

We consider square arrays of Cd$_3$As$_2$ with a relative permittivity $\varepsilon$, thickness of 0.5 $\mu$m [see Fig. 1(a)]. Periodic boundary conditions are applied along both $x$ and $y$ directions with periodicity $P_x = P_y = 86$ $\mu$m. The gap between adjacent square is 36 $\mu$m. The coordinate system is defined such that $x$ and $y$ directions are lying in the plane of the square which has a width of $a = 50$ $\mu$m [Fig. 1(b)]. The finite-difference-time-domain (FDTD) method is employed to calculate transmission spectra, phase, amplitude and EFDs, which reveal the resonance mechanisms and transmission properties of the device. The polarization angle is defined as $\varphi$ as shown in Fig. 1(b). Thus, $\varphi = 0^\circ$ and $\varphi = 90^\circ$ correspond to TM- and TE-polarized wave, respectively. A linearly-polarized plane wave at normal incidence is considered. To avoid nonphysical reflections of outgoing electromagnetic waves from the grid boundaries, a perfectly matched layer of thickness of 0.5 $\mu$m and a length of $2a$ is introduced between adjacent square to circumvent the need of fabricating complex chiral photonic devices.

For computational simplicity, air is assumed to be the background.

The optical anisotropy of Cd$_3$As$_2$ is modelled based on a previously developed optical conductivity model obtained from Kubo formula. The semiclassical intraband and quantum mechanical interband optical conductivities are determined, respectively, as

$$\sigma_{ii}^{\text{intra}}(\omega) = \frac{g e^2 v_i}{6\pi^2 \hbar^3 v_x v_y} \frac{\tau}{i \omega T - 1} \int_{-\infty}^{+\infty} \frac{\partial f_D(\varepsilon)}{\partial \varepsilon} \varepsilon^2 d\varepsilon \quad (1a)$$

$$\sigma_{ii}^{\text{inter}}(\omega) = \frac{i g e^2 v_i v_j}{3 \pi^2 \hbar^2 v_x v_y} \int_{0}^{+\infty} \frac{G(\varepsilon) \varepsilon}{\hbar^2 (\omega + i0^+)^2 - 4 \varepsilon^2} d\varepsilon, \quad (1b)$$

where $g = 4$ is the degeneracy factor, $i = x, y, z$ denotes the three orthogonal lattice directions, $v_i \neq v_j \neq v_k$ are the Fermi velocity parameter in the $i, j, k$-direction, respectively, $G(\varepsilon) = f_D(-\varepsilon) - f_D(\varepsilon) = \text{sinh}(\beta\varepsilon)/(\cosh(\beta\varepsilon) + \cosh(\beta\mu))$, $f_D(\varepsilon)$ is the equilibrium Fermi-Dirac distribution function, $\mu = 50$ meV is the Fermi level, $\beta = 1/k_BT$ is the inverse thermal energy, and $T = 300$ K at room temperature and the scattering time constant is assumed to be $\tau \approx 450$ fs. The permittivity can be calculated as $\varepsilon_{ii}(\omega) = 1 + i \sigma_{ii}^{\text{tot}}(\omega)/\omega \epsilon_0$, where $\epsilon_0$ is the permittivity of free space, and $\sigma_{ii}^{\text{tot}}(\omega) = \sigma_{ii}^{\text{intra}}(\omega) + \sigma_{ii}^{\text{inter}}(\omega)$. For Cd$_3$As$_2$, the Fermi velocity parameter is highly anisotropic ($v_x$, $v_y$, $v_z$) = (1.28, 1.30, 0.33) $\times 10^6$ m/s. In this case, the permittivity exhibits a strong directional dependence with $\varepsilon_{xx} \neq \varepsilon_{yy} \neq \varepsilon_{zz}$ in general. To highlight the significance of optical anisotropy of TDSM, we also perform benchmark studies using the isotropic optical model of TDSM. As demonstrated below, the C$_4$-symmetric metasurface studied here exhibits radically different optical responses when the optical anisotropy is omitted, thus highlighting the importance and necessity of incorporating the anisotropic permittivity in the computational designs of TDSM-based photonic devices.

In symmetric structure with isotropic materials, super-radiant or bright modes couple strongly to the incident field, producing broad and lossy resonances. In the presence of geometrical asymmetry, sub-radiant or dark modes can be excited. These dark mode resonances couple weakly to the free space and lead to high values of quality factor ($Q$-factor). Fano-type resonance caused by symmetry breaking can result in an asymmetric spectral profile. In relevance to this, we first focus on the optical response of Cd$_3$As$_2$ metasurface outlined in Fig. 1(a) under the oversimplified isotropic approximation of $\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz}$. In this case, the transmission response is identical under both TE- and TM-polarized wave [Fig. 2(a) and the inset for the corresponding EFDs]. In contrast, when the optical anisotropy is included, the trans-

![FIG. 1. Device design of the Topological Dirac Semimetal Cd$_3$As$_2$ metasurface. (a) Schematic 3D view of the proposed TDSM model system. The Cd$_3$As$_2$ layer has a thickness of 0.5 $\mu$m. (b) One-pixel cell structure of the square-lattice-based metasurface. The pixels are arranged with periods $P_x = P_y = 86\mu$m. The squares have a length of $a = 50$ $\mu$m. Polarization angle is defined as $\varphi$, with $\varphi = 0^\circ$ and $\varphi = 90^\circ$ correspond to TM and TE wave, respectively. A linearly-polarized plane wave impinges on the top of the system and propagates perpendicular to the $xy$-plane.](image-url)
mission spectra exhibit completely different line shapes for TE- and TM-polarized waves [Fig. 2(b)]. For a better insight into the nature of these resonant modes, we plot the out-of-plane EFDs (i.e. $E_z$) at each resonance mode [Figs. 2(c) and 2(d)]. The EFDs of the first four modes, labelled as $\mathbb{1}$-$\mathbb{4}$ in Fig. 2(b), are shown in Fig. 2(c) for TE-polarized wave. A broadband feature occurs at about 0.88 THz [labeled as $\mathbb{1}$] corresponds to the super-radiant mode that couples strongly to the free space. The radiation field of the dipole interferes strongly, resulting in the occurrence of various symmetric dipole modes [see Fig. 2(c)]. In addition to these dipolar modes, four narrower asymmetric resonance modes, labeled as $\mathbb{5}$-$\mathbb{8}$ in Fig. 2(b), which correspond to resonances with very low radiation losses and high $Q$ factor, are also present under the TM-polarized wave. Furthermore, the symmetric modes in Fig. 2(c) display a net dipole moment. Such net dipole moment is completely absent in the asymmetric modes in Fig. 2(d). Importantly, Fig. 2 reveals the very different nature of the resonances under TE- and TM-polarized incidence. Such phenomenon is a direct consequence of the anisotropic permittivity of optically anisotropic Cd$_3$As$_2$. Thus, by exciting these different spectral responses, one can switch between the symmetric and antisymmetric effects simply through rotating the polarization direction of the incident light.

The device performance parameters, namely the resonant frequency, full width at half maximum (FWHM) and $Q$-factor, are listed in Table I for the metasurface simulated under both isotropic and anisotropic models. Interestingly, the FWHM and $Q$-factor of isotropic approximation is significantly smaller than that of the anisotropic optical model. The exceptionally high $Q$-factor, reaching as high as $10^2$ to $10^3$, obtained from the anisotropic model suggests an excellent performance in THz region failed to be captured under the isotropic approximation. The underlying reason of the better performance is due to the significantly Fermi velocity of $1.30 \times 10^6$ m/s along the $y$ crystal direction of Cd$_3$As$_2$ is significantly larger than that commonly employed in the isotropic approximation of $1.0 \times 10^6$ m/s which directly influences the $Q$-factor. In general, larger Fermi velocity constant produce the resonances with a larger $Q$ factor. This can be seen from the optical conductivity expression in Eq. (1). The $i$-directional conductivity is generally inversely proportional to $v_{j,k}$. A larger Fermi velocity constant thus suppresses the real part of the optical conductivity and, correspondingly, the imaginary part of the dielectric permittivity, $\Im[\varepsilon(\omega)]$. The suppression of $\Im[\varepsilon(\omega)]$ results in the exceptionally large $Q$-factor. The narrow FWHM and high $Q$-factor typically occurs for higher modes $\mathbb{5}$-$\mathbb{8}$, suggesting that these sharp peaks and dips of Fano resonance may be harnessed for high-sensitivity biosensors applications. Importantly,
TABLE I. Comparison of isotropic and anisotropic modelling of Cd$_3$As$_2$ square-lattice metasurface. The resonant frequency, FWHM, Q-factor and the corresponding mode label displayed in Fig. 2 are shown.

| Systems          | Resonant frequency (THz) | Mode label | FWHM (THz) | Q-factor |
|------------------|--------------------------|------------|------------|----------|
| isotropic TDSM (TE) | 2.76                     | n.a.       | 1.17       | 2.36     |
| isotropic TDSM (TM) | 2.76                     | n.a.       | 1.17       | 2.36     |
| anisotropic TDSM (TE) | 0.88                     | 1          | 0.17       | 5.17     |
|                  | 1.91                     | 2          | 0.01       | 191      |
|                  | 2.53                     | 3          | 0.04       | 632.5    |
|                  | 2.96                     | 4          | 0.03       | 986.7    |
| anisotropic TDSM (TM) | 2.21                     | 5          | 0.03       | 73.6     |
|                  | 2.73                     | 6          | 0.019      | 143.7    |
|                  | 3.06                     | 7          | 0.08       | 382.5    |
|                  | 3.36                     | 8          | 0.07       | 480      |

FIG. 3. Transmission spectra for different polarization angles of the incident wave. The modes labelled 1 to 8 here are the same as that labelled in Fig. 2. As $\varphi$ increases from 0° towards 90°, the sharp transmission peaks corresponding to the antisymmetric modes (denoted by the labels 1 to 8 in Fig. 3) recede gradually while that corresponding to symmetric modes (denoted by the labels 9 to 10 in Fig. 3) become increasingly prominent, showing a direct consequence of the optical dichroism of Cd$_3$As$_2$.

The device performance characteristics outlined in Table I suggest that the anisotropic optical model of TDSM better captures the superior application potential of Cd$_3$As$_2$ in THz waves modulation, as compared to the less accurate, or oversimplified, isotropic optical model.

To gain an understanding on how different polarization angles can influence the transmission intensity and spectra position, the optical response at varying $\varphi$ is calculated. We calculate the transmission spectra of the system at several polarization angles ranging from $\varphi = 0°$ to $\varphi = 90°$ with 10° steps. Two different processes are responsible for the observed variation in transmission spectra shown in Fig. 3. The incident light with an arbitrary polarization angle $\varphi$ can be decomposed into two components, namely the parallel ($\varphi = 0°$) and perpendicular ($\varphi = 90°$) polarization components. For an incident wave with $\varphi = 0°$ and $\varphi = 90°$, only the antisymmetric and the symmetric modes are excited, respectively. However, when $\varphi$ is intermediate between 0° and 90°, the spectra response exhibit a mixture of the symmetric and antisymmetric modes. As $\varphi$ increases from 0° towards 90°, the sharp transmission peaks corresponding
FIG. 4. Transmission amplitude and relative phase delay of the isotropic and anisotropic TDSM metasurface. (a) Transmission amplitudes, $T_{xx}$ and $T_{yy}$, of the isotropic models of TDSM metasurface as a function of frequency, where $T_{xx}$ and $T_{yy}$ are the x-polarized transmission under x-polarized incidence, and y-polarized transmission under y-polarized incidence, respectively. (b) Phase information, $\phi_{xx}$, $\phi_{yy}$, and the relative phase delay $\Delta \phi$ of the isotropic models of TDSM as a function of frequency, where $\phi_{xx}$ and $\phi_{yy}$ are the phases of the transmitted waves along the x- and y-directions, respectively. (c) Schematic illustration of THz wave transmission across an isotropic TDSM metasurface in which polarization conversion effect is absent. (d) and (e), same as (a) and (b), but for the case of optically anisotropic TDSM. (f) Schematic illustration of the linear-to-circular polarization conversion in an optically dichroic TDSM metasurface.

to the antisymmetric modes (denoted by the labels ① to ⑤ in Fig. 3) recede gradually while that corresponding to symmetric modes (denoted by the labels ⑥ to ⑧ in Fig. 3) become increasingly prominent.

The $\varphi$-tunable symmetric-to-antisymmetric mode transition reveals an intriguing behavior of optically anisotropic TDSM metasurface. The transmitted electromagnetic waves can be dramatically modulated by changing the polarization angle of a linearly polarized incident wave even though the metausrface is composed of highly symmetric square lattices. This behavior is a direct consequence of the optical dichroism of Cd$_3$As$_2$ and is completely missed out in the simplistic isotropic optical conductivity model of TDSM.

The occurrence of highly asymmetric spectra response from a highly symmetric structure reveals the potential of Cd$_3$As$_2$ – an optically anisotropic TDSM – in achieving efficient polarization conversion without involving complex chiral or supercell structures that are challenging to fabricate experimentally. At normal incidence, the incident electric field can be represented by $\vec{E}_{in} = (E_x \hat{x} + E_y \hat{y})e^{i(\omega z/c + \omega t)}$, where $E_x$ and $E_y$ are the electric field components along the x and y directions, respectively. After traversing a high-symmetry structure and isotropic system, the transmitted electric field becomes $\vec{E}_{tiso} = t_x E_x \hat{x} + E_y \hat{y})e^{i(\omega z/c + \omega t)}$, where $t_x$ is the transmission coefficient, and the transmitted electric field is insensitive to the relative contributions between $E_x$ and $E_y$ for a given incident wave. In contrast, for an anisotropic system with $\varepsilon_{xx} \neq \varepsilon_{yy} \neq \varepsilon_{zz}$, the transmission coefficients are different for incident waves polarized along the x and y directions. The transmitted electric field becomes $\vec{E}_{taniso} = (t_x E_x \hat{x} + t_y E_y \hat{y})e^{i(\omega z/c + \omega t)}$ with directional-dependent transmission coefficients, $t_x$ and $t_y$. As $t_x \neq t_y$ in general, the relative composition of $E_x$ and $E_y$ of the incident wave can dramatically modulates the transmitted wave. As demonstrated below, the optical anisotropy of TDSM can be readily harnessed to achieve linear-to-circular polarization conversion of an incident THz wave – a behavior not achievable under the isotropic model of TDSM.

The phase and amplitude play a crucial role in determining the polarization state of the transmitted wave. To characterize the polarization conversion operation of...
TDMS, we calculate the phase and amplitude of the transmission spectra in Fig. 4. Here, polarization conversion is related to the relative phase delay between the $x$- and $y$-components of the transmitted wave. We first show that, under the isotropic approximation, TDMS is not capable of polarization conversion. In this case, the transmission amplitudes, $T_{xx}$ and $T_{yy}$ [Fig. 4(a)] and the phases, $\phi_{xx}$ and $\phi_{yy}$ of the $x$- and $y$-components of the transmitted wave are completely identical [Fig. 4(b)]. Thus, the transmitted wave retains the polarization state of the incident wave in an isotropic TDMS model [Fig. 4(c)], which is expected due to the highly-symmetric nature of the square lattices exhibiting a $C_4$ rotational symmetry perpendicular to the optical axis of the normal incidence. In contrast, transmission amplitudes are drastically different for TE- and TM-polarized waves in the case of anisotropic TDMS [Fig. 4(d)]. The corresponding $\phi_{xx}$ and $\phi_{yy}$ exhibit contrasting dispersion between the $x$- and $y$-components of the transmitted waves [Fig. 4(e)]. Aside from amplitude parameter, the phase difference defined as $\Delta \phi = \phi_{xx} - \phi_{yy}$ is another crucial role for the polarization conversion. As shown in Fig. 4(e), the phase difference distinctly indicate a strongly nonlinear curve. Specifically, the mode $\Omega$ located at 0.88 THz lifts the phase dispersion curve and a phase shift of $\pi$ occurs. Intriguingly, the right-side tail of mode $\Omega$ (0.88 THz) and the left-side tail of mode $\Omega$ (1.91 THz) makes a close-to-linear dispersion at off-resonance frequencies between the two modes. Simultaneously, the same tendency appears between other adjacent resonance modes with different phase jump. Such a nonlinear phase dispersion related to the polarization state of transmission wave provides a possibility of efficient-broadband polarization conversion. Importantly, the relative phase delay is limited to the range of $-\pi/2$ and $+\pi/2$, covers multiple special values, such as $-\pi/2$, 0 and $\pi/2$, thus indicating that multiple polarization states (i.e. circularly-, linearly-, elliptically-polarized wave) can be achieved by appropriately matching the transmitted wave amplitudes and the relative phase delay. For example, linear-to-circular polarization conversion, akin to the polarization conversion of a quarter-wave plate, can be achieved with the simultaneous fulfillment of $T_{xx} = T_{yy}$ and $\Delta \phi = \pm \pi/2$ which generates two co-propagating wave components of equal amplitudes of orthogonal linear polarizations and phase-shifted by a quarter-wavelength [Fig. 4(f)]. Within the frequency window of 0.5 THz to 3.5 THz, there are four operation frequencies [labelled as $P_1$ to $P_4$ in Figs. 4(d) and 4(e)] capable of producing linear-to-circular polarization conversion.

Apart from linear-to-circular polarization conversion, linear-to-elliptical polarization conversion can also be achieved under the conditions of $\Delta \phi = n \pi/2$ but with $T_{xx} \neq T_{yy}$. Multiple of such operating frequencies are identified as labelled by the red circles in Figs. 4(d) and 4(e). Furthermore, between the two resonances frequencies of 0.88 THz to 1.91 THz, an expansive region of nearly constant phase delay of $\sim 0.2\pi$ is present, suggesting a broadband frequency windows capable of producing linear-to-elliptical polarization conversion. Importantly, despite the relatively simple geometry of the square-lattice-based metasurface, the optical dichroism of Cd$_3$As$_2$ enables such metasurface to perform various polarization conversions in THz regime. This highlights the importance and unique features of optically dichroic TDMS not captured by the isotropic optical model commonly employed in the literature. Finally, we note that the geometrical parameters of the Cd$_3$As$_2$ metasurface can be further optimized the achieve desired polarization conversion performance.

In conclusion, we reported the optical response and polarization conversion operation of a $C_4$ symmetric metasurface composed of Cd$_3$As$_2$ square lattices. By explicitly taking into account the optical dichroism of Cd$_3$As$_2$ using an optical conductivity model obtained from the Kubo formula, we found that the metasurface exhibits strongly asymmetric transmission spectra sensitively influenced by the polarization angle of the incident waves. Such directional-dependent transmission dramatically affects the optical response of the metasurface and is not captured by the isotropic TDMS model. Intriguingly, the optical dichroism of Cd$_3$As$_2$ can be harnessed to achieve linear-to-circular and linear-to-elliptical polarization conversion of terahertz waves using a simple square-lattice metasurface, thus circumventing the need of complex device morphology, such as chiral or multilayer structures. These findings revealed the shortcomings of the commonly employed isotropic optical model of TDMS in the computational modeling of TDMS-based photonic devices, and highlighted the unique strength of optically anisotropic topological Dirac semimetal in THz waves polarization conversion applications without the need of complex device morphology.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors declare that there are no conflicts of interest.

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable
request.

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