Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

All-dielectric terahertz metasurface with dual-functional polarization manipulation for orthogonal polarization states

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S1: Equation derivation for the bifunctional waveplate

In the main text, we have derived the electric field of the transmitted wave under RCP (LCP) incidence for the basic unit constructed from meta-atom A and meta-atom B. For simplicity, according to equation (8), only one of the solutions satisfying this equation is considered for analysis here:

$$\Delta\varphi_1/2=\Delta\varphi_1/2=\pi/4 \qquad \text{(S1).}$$

The basic unit only engenders the co-polarized wave under the incidence of LCP wave, indicating that the RCP components generated by the meta-atom A and the meta-atom B exist interference cancellation. Then from equation (5), it can be concluded that:

$$\sum\varphi_1/2-\pi/2-2\theta_1=\sum\varphi_2/2-\pi/2-2\theta_2+\pi \qquad \text{(S2).}$$

In addition, the basic unit will generate x-LP waves under RCP incidence, then there will be two possible solutions to equation (7), one of which is:

$$\begin{cases}\sum\varphi_1/2-\pi/2+2\theta_1=\sum\varphi_1/2\\ \sum\varphi_2/2-\pi/2+2\theta_2=\sum\varphi_2/2\end{cases} \qquad \text{(S3).}$$

Obviously, equation (S3) is not tenable. Otherwise, if both equation (S2) and equation (S3) are satisfied, the basic unit will not generate transmitted waves under LCP incidence. Therefore, the other solution can be expressed as:

$$\begin{cases}\sum\varphi_1/2-\pi/2+2\theta_1=\sum\varphi_2/2\\ \sum\varphi_2/2-\pi/2+2\theta_2=\sum\varphi_1/2\end{cases} \qquad \text{(S4).}$$

Simultaneous equations (S1), (S2) and (S3) can be solved to obtain the following results: $\sum\varphi_1=\sum\varphi_2+\pi/3$, $\theta_1=\pi/12$ and $\theta_2=5\pi/12$. Finally, the conditions that meta-atom A and meta-atom B need to meet can be obtained: $\Delta\varphi_1/2=\Delta\varphi_2/2=\pi/4$, $\varphi_{xx1}=\varphi_{xx2}+\pi/3$, $\theta_1=\pi/12$ and $\theta_2=5\pi/12$.

S2: Meta-atom A and meta-atom B for construction of the bifunctional waveplate

In the previous section, the conditions that meta-atom A and meta-atom B need to meet have been obtained through theoretical derivation. In this section, simulation software the CST Studio Suite will be used to calculate the results under different geometric parameters, and then the required meta-atoms will be intellectually selected. As shown in Figure 1b (see main text), the fast and slow axes of the elliptical pillar are b and a, respectively, and its thickness is 300 μm. The thickness of the substrate is 700 μm, and its period is 120 μm. With this, under LP incidence, the transmission coefficients corresponding to different a and b are obtained by simulation (see **Figure S1**), where the operating frequency is uniformly 0.8 THz. Herein, Figures S1a and S1b show amplitude and phase delay along x-axis under x-LP incidence, while the amplitude and phase delay along the y-axis under y-LP incidence are plotted in Figures S1c and S1d.

Obviously, for meta-atom A and meta-atom B, the phase difference propagating along the x- and y-directions is π/2. Afterwards, according to the requirements mentioned in section **S1**, a suitable set of parameters for meta-atom A and atom B are selected: a_1 = 40 μm, b_1 = 53 μm, θ_1 = π/12, a_2 = 37 μm, b_2 = 49 μm and θ_2 = 5π/12.

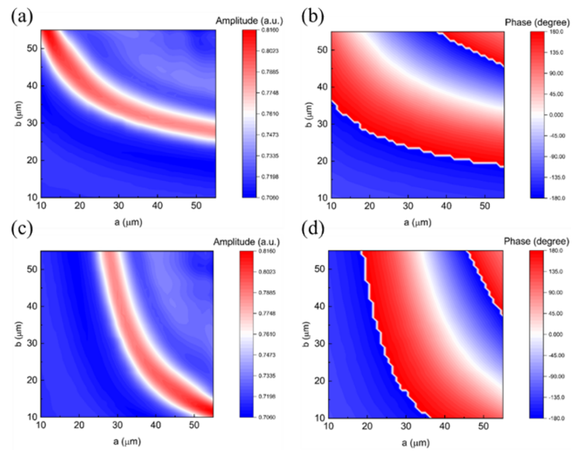

Figure S1 (a-d) Schematic of the amplitudes and phase delays along x-axis (y-axis) under x-LP (y-LP) incidence at 0.8 THz.

S3: The basic unit for constructing the near-field imaging metasurface

In this section, we derive a basic unit with a specific function through theoretical analysis: the basic unit can generate a transmitted x-LP wave under LCP incidence, and will engender the co-polarized outgoing wave under RCP illumination. Using a derivation scheme similar to that in section **S1**, here meta-atom A and meta-atom B also need to satisfy equation (S1). Next, we discuss the results for RCP and LCP incidences, respectively. For RCP incidence, it can be concluded according to equation (7):

$$\sum\varphi_1/2-\pi/2+2\theta_1=\sum\varphi_2/2-\pi/2+2\theta_2+\pi \qquad \text{(S5)},$$

which illustrates that in the case of RCP incidence, the LCP components yielded by meta-atom A and meta-atom B interfere destructively. Meanwhile, for LCP incidence, two possible solutions can also be obtained according to equation (5). One set of solutions is:

$$\begin{cases}\sum\varphi_1/2-\pi/2-2\theta_1=\sum\varphi_1/2\\ \sum\varphi_2/2-\pi/2-2\theta_2=\sum\varphi_2/2\end{cases} \qquad \text{(S6)},$$

which is similar to the results of the previous discussion, so this case does not exist. Then, another possible set of solutions is:

$$\begin{cases}\sum\varphi_1/2-\pi/2-2\theta_1=\sum\varphi_2/2\\ \sum\varphi_2/2-\pi/2-2\theta_2=\sum\varphi_1/2\end{cases} \qquad \text{(S7)}.$$

Combined with equations (S1), (S5) and (S7), the conditions required for the construction of the near-field imaging metasurface are obtained: $\Delta\varphi_1/2$ = $\Delta\varphi_2/2$ = π/4, φ_{xx1} = φ_{xx2}+π/3, θ_1 = -π/12 and θ_2 = -5π/12. Thus, according to section **S2**, we can obtain the geometric parameters of the basic unit composed of meta-atom A and meta-atom B: a_1 = 40 μm, b_1 = 53 μm, θ_1 = -π/12, a_2 = 37 μm, b_2 = 49 μm and θ_2 = -5π/12. Besides, in the main text, we define the basic unit in section **S1** as Ent C, and the basic unit in this section as Ent D.

S4: The basic unit for constructing the metasurface zone plate

Since the designed metasurface zone plate produces a focused co-polarized wave under LCP incidence and a focused x-LP wave under RCP illumination, it can be determined according to equation (12a):

$$\sum\varphi_1/2-\pi/2-2\theta_1=\sum\varphi_2/2+\pi/2-2\theta_2+\pi \qquad \text{(S8)}.$$

Likewise, for RCP incidence, we can obtain a set of solutions from equation (12b):

$$\begin{cases} \sum\varphi_1/2 - \pi/2 + 2\theta_1 = \sum\varphi_1/2 \\ \sum\varphi_2/2 + \pi/2 + 2\theta_2 = \sum\varphi_2/2 \end{cases} \quad \text{(S9).}$$

Thus, θ_1 and θ_2 are equal to π/4 and -π/4, respectively. Once equations (S8) and (S9) are substituted into equation (12a), it can be concluded that the designed metasurface zone plate does not generate transmitted waves under LCP incidence, which is contrary to the original intention of the design. Therefore, we discuss another set of solutions to equation (12b):

$$\begin{cases} \sum\varphi_1/2 - \pi/2 + 2\theta_1 = \sum\varphi_2/2 \\ \sum\varphi_2/2 + \pi/2 + 2\theta_2 = \sum\varphi_1/2 \end{cases} \quad \text{(S10).}$$

Solving the equations (S1), (S8) and (S10) to obtain the final results: $\Delta\varphi_1/2 = \Delta\varphi_2/2 = \pi/4$, $\varphi_{xx1} = \varphi_{xx2}-2\pi/3$, $\theta_1 = \pi/12$ and $\theta_2 = 5\pi/12$. The specific parameters of meta-atom A and meta-atom B in section **2.3** are obtained by parameter scanning.

S5: Experimental Section

Numerical simulations: The simulated results of elliptical pillars with different geometric parameters are obtained by using the software CST Studio Suite (2019). After building the elliptical pillar model, we set the x- and y-directions as periodic boundaries, the boundaries along the z direction are open, and the frequency range is set to 0.6-1.2 THz. The probe is then placed at the appropriate location to detect the corresponding transmission amplitude and phase generated by the elliptical pillar under orthogonal LP incidence, thereby determining the desired unit. Finally, in order to obtain the transmission spectrum or electric field distribution of the designed metasurface when a specific polarized wave is incident, we set the x-, y-, and z-directions in the boundary as open boundaries. It should be noted that the electric field distribution can be obtained through the post-processing module of the software CST Studio Suite.

Sample Fabrication: We combine standard UV lithography and inductively coupled plasma (ICP) etching to process the designed all-dielectric terahertz metasurfaces. Here, a 4-inch silicon wafer with a thickness of 1 mm is used for sample fabricating. The specific process flow is as follows: (1) Clean the silicon wafer to remove dust and various contaminants on the surface of the silicon wafer; (2) Spin-coat positive photoresist (AZ4620) and pre-bake to obtain a thin photoresist film; (3) Align the mask with the silicon wafer and expose it, and then develop it; (4) The exposed silicon is etched and etched by ICP ion etching machine (STS MULTIPLEX ASE-HRMICP ETCHER); (5) The photoresist is removed with acetone, then the silicon wafer is cleaned with alcohol and deionized water and finally dried.

The terahertz digital holographic imaging system (see **Figure 2**): In such system, the sample is placed between parabolic mirror (PM) and ZnTe, where PM can collimate terahertz wave with a diameter of about 4 cm and ZnTe detector crystal receives terahertz wave passing through the sample. After the probe beam is reflected to the probe crystal (ZnTe) by the beam splitter (BS), the Pockels effect in the ZnTe detection crystal is excited by terahertz field and the polarization of the probe beam is modulated. Finally, the polarization modulated probe beam is captured by a CCD to generate terahertz images.

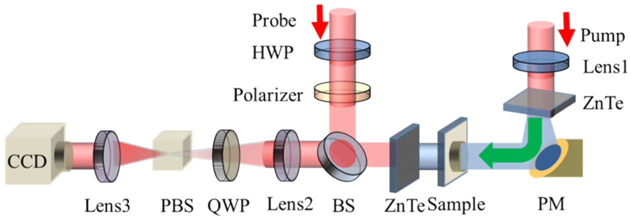

Figure S2 Schematics of the THz digital holographic imaging system. The sample is placed between PM and ZnTe, where PM is the abbreviation of parabolic mirror. HWP: Half-wave plate, QWP: quarter-wave plate, PBS: polarization beam splitter.