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All-dielectric KTiOPO$_4$ metasurfaces based on multipolar resonances in the terahertz region

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Abstract: We employ ferroelectrics to study the multipolar scattering in all-dielectric metasurfaces based on KTiOPO$_4$ (KTP) micro-disks for efficient manipulation of electromagnetic waves in the THz spectral region (0.6-1.5 THz). By adjusting the aspect ratio of the disks near the multipolar resonances, we show that the KTP disk array can form a multifunctional metasurface that covers the entire range of the electromagnetic response with resonantly enhanced anisotropic properties. The proposed ferroelectric metasurfaces will provide a versatile platform to manipulate THz waves, and open possibilities to monolithically combine it with THz generation.

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1. Introduction

Metasurfaces composed of subwavelength resonant elements are the two-dimensional analogue of metamaterials. By locally modifying the amplitude [1–5], polarization [6–10] and phase [11–17] of the incident light at the metasurface, one can control the wavefront to implement complex functionalities in a subwavelength-thin optical element.

All-dielectric metasurfaces [1–8, 13–19] have recently been adopted as alternatives to their metallic counterparts [9–12, 20–22] in the visible and the infrared regions. Their full phase coverage originating from the exhibition of both electric and magnetic resonances [23–27] enables a highly efficient light manipulation in waveplates [6] and polarizers [7] and holograms [13–16]. Most of the all-dielectric metasurfaces are made of narrow bandgap materials [18], such as Si and Ge, due to their high indices of refraction as well as low loss. For the same reason, Si was also used in the recent demonstration of all-dielectric metasurfaces in the terahertz (THz) frequency range [4, 5, 17], while the designs of the metasurfaces for THz waves are still largely focused on metallic structures [11, 22].

Searching for dielectrics with a high dielectric constant to support the excitation of high-quality multipolar resonances in the THz region, one could also consider ferroelectric crystals, such as LiNbO₃, LiTaO₃, KTiOAsO₄ or KTiOPO₄ (KTP). For example, KTP provides a relatively high dielectric constant e.g. $\varepsilon_x \approx \varepsilon_y \approx 11$, $\varepsilon_z \approx 16$ at 1.5 THz [28]. KTP and its isomorphs are well-established nonlinear optical materials with strong 2nd-order nonlinearities that can be engineered via $\chi^{(2)}$ structuring. Similar to other ferroelectrics, KTP is also characterized by a strong coupling of the THz electromagnetic waves to the transversal optical (TO) phonon modes, which gives rise to phonon-polariton waves propagating in the crystal. Employing such polaritonic material to design all-dielectric metasurfaces, one might even combine the manipulation of THz wave with its generation [29–32], and realize compact THz devices with small footprints. Nevertheless, the strong absorption that is present near the phonon resonances has so far hindered the applications of ferroelectric crystals for constructing efficient all-dielectric metasurfaces. In the case of KTP, however, the absorption can, in fact, be comparable to that of the existing applications using Si near the band-edge at room temperature [14,15,19], if we utilize the spectral window below 1.5 THz to avoid the strongest phonon lines. The absorption in KTP is typically pronounced along the titanyl bonds in the crystal z-axis with the absorption coefficients of $\alpha_x \approx \alpha_y < 15 \text{ cm}^{-1}$, $\alpha_z < 50 \text{ cm}^{-1}$, that are well-maintained below 1.5 THz. The applicable bandwidth in KTP may be attainable even in a higher THz frequency range as THz parametric oscillators have been demonstrated in KTP and its isomorphs reaching 6.2 THz [32–34]. In contrast, THz generation using LiNbO₃ has been limited by absorption to the range below 3 THz [35]. In the semi-transparent THz spectral range, the absorption can further be mitigated by employing subwavelength thickness in the structural design.

In this work, we employ the ferroelectric crystal, KTP, to construct all-dielectric metasurfaces for efficient manipulation of electromagnetic waves in the THz range (0.6 – 1.5 THz) based on the anisotropic multipolar interference. The strong birefringence for x-cut (or y-cut) KTP naturally results in a different electromagnetic response under each polarization, which offers more degrees of freedom in the manipulation of the incident THz waves. We first elucidate the unique anisotropic multipolar scattering behavior in a single KTP disk. Adjusting the aspect ratio of the disks in a square array, we show that the array can form a uniform metasurface whose electromagnetic functionality could be easily changed from transparent films to electric mirrors, magnetic mirrors [3], negative index materials [36] or near-zero index materials [37, 38] in the THz range. In this case, the designed metasurface can exhibit a multifunctional behavior under different polarizations as the intrinsic anisotropy
of KTP is significantly enhanced near the multipolar resonances. Finally, adopting a nonuniform distribution in the size of KTP disks, we propose a chirped metasurface that shows an anisotropic deflection behavior near the multipolar resonances. This can be used to steer the incident THz waves with a strong polarization dependence.

2. Anisotropic scattering behavior of a single KTP disk

KTP metasurfaces in our study are modeled by the finite-difference time-domain (FDTD) method (Lumerical FDTD Solutions, version 8.15.697) with the refractive index of KTP taken from Antsygin’s work [28] (see Appendix A for more detail). The spectral range in the simulation covers from 0.6 THz to 1.5 THz, where KTP maintains relatively low loss in the THz region. The overall system is illuminated by plane waves propagating along the $x$-axis, where the coordinate of the system follows the crystal axes. We adopt a total-field scattered-field (TFSF) formulation to study the anisotropic scattering and absorption properties of the KTP structures in FDTD.

We first elucidate the resonant scattering properties of a single KTP disk under different polarizations by conducting multipolar decompositions of the total scattering cross-section in vacuum [26]. The multipole moments can be calculated from the electric field distribution in the KTP disk as follows,

$$ p = \varepsilon_0 (\varepsilon_d - \varepsilon_r) \int E(r) dV $$

$$ m = \frac{i\omega\varepsilon_0 (\varepsilon_d - \varepsilon_r)}{2\nu_d} \int [r \times E(r)] dV $$

$$ Q_{\alpha\beta} = \frac{\varepsilon_0 (\varepsilon_d - \varepsilon_r)}{2} \int \left\{ r_\alpha E_\beta + r_\beta E_\alpha - \frac{2}{3} [r \cdot E(r)] \delta_{\alpha\beta} \right\} dV $$

$$ M_{\alpha\beta} = \frac{i\omega\varepsilon_0 (\varepsilon_d - \varepsilon_r)}{3\nu_d} \int \left\{ [r \times E(r)]_\alpha r_\beta + [r \times E(r)]_\beta r_\alpha \right\} dV $$

The definitions of the parameters used here are summarized in the Table 1.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P$</td>
<td>Electric dipole moment</td>
</tr>
<tr>
<td>$m$</td>
<td>Magnetic dipole moment</td>
</tr>
<tr>
<td>$Q_{\alpha\beta}$</td>
<td>Electric quadrupole tensors</td>
</tr>
<tr>
<td>$M_{\alpha\beta}$</td>
<td>Magnetic quadrupole tensors</td>
</tr>
<tr>
<td>$\alpha, \beta$</td>
<td>Cartesian components in the coordinate system</td>
</tr>
<tr>
<td>$\varepsilon_d$</td>
<td>Relative permittivity of a dielectric, i.e. KTP</td>
</tr>
<tr>
<td>$\varepsilon_r$</td>
<td>Relative permittivity of vacuum</td>
</tr>
<tr>
<td>$\nu_d$</td>
<td>The speed of light in vacuum</td>
</tr>
<tr>
<td>$E$</td>
<td>The electric field extracted from FDTD simulation</td>
</tr>
</tbody>
</table>

Figures 1(a) and 1(b) show that the sum of multipolar scattering cross-sections is in good agreement with the total scattering cross-section calculated by FDTD simulation along the $y$- and $z$-axis, respectively. This validates our formalism where the scattering behavior of the KTP disk is projected into that of an electric dipole, a magnetic dipole, an electric quadrupole and a magnetic quadrupole. The insets in Figs. 1(a) and 1(b) describe the electric field distributions at the corresponding resonances inside the disk, of which cross-section is chosen to be perpendicular to the incident magnetic field to show that the typical displacement current loop can be observed at each magnetic dipole resonance near the wavelength of 270 μm and 300 μm, respectively.
Fig. 1. Anisotropic scattering and absorption properties of a single KTP disk with $h = 60 \text{ µm}$ and $d = 80 \text{ µm}$ in vacuum. The total scattering cross-section is projected into an electric dipole ($\text{ED}$, green dashed line), a magnetic dipole ($\text{MD}$, blue dotted line), an electric quadrupole ($\text{EQ}$, cyan dash dotted line) and a magnetic quadrupole ($\text{MQ}$, magenta dash dotted line) under the normal incidence of (a) $\gamma$-polarized or (b) $\beta$-polarized THz plane waves. The black solid line represents the result from our FDTD simulation for the total scattering cross-section, while the red dashed line shows the sum of the multipole scattering cross-sections. The insets describe the normalized electric field distribution at each dipole resonances in the $x$-$y$ ($x$-$z$) plane under the $\gamma$-polarized ($\beta$-polarized) illumination. (c) Calculated absorption cross-sections under the two orthogonal polarization states. The calculated cross-sections are normalized to the physical area of the disk, i.e. $\pi (d/2)^2$.

In the comparison between Figs. 1(a) and 1(b), the resonant scattering behaviors under the two orthogonal polarizations appear to be similar to each other at the multipolar resonances, apart from the fact that there is a noticeable spectral red-shift in Fig. 1(b) due to the higher refractive index along the $z$-axis in KTP. In Fig. 1(c), however, the absorption cross-section along the $\gamma$-axis is clearly distinguished from the one along the $z$-axis, showing that the KTP disk is significantly less absorptive under the $\gamma$-polarized incident electric field.

3. A uniform metasurface with a square array of KTP disks

Based on the knowledge of the anisotropic scattering and absorption properties of the single KTP disk, we propose a uniform metasurface formed by a square array of KTP disks on a polymer substrate, as depicted in Fig. 2(a). Each KTP disk has the fixed height of $h = 60 \text{ µm}$ and the diameter $d$ that is varied from $60 \text{ µm}$ to $200 \text{ µm}$. In order to obtain a high scattering efficiency of the array and simultaneously maintain the high-quality resonances at each disk, the gap between the nearest disks is optimized and fixed to $g = 60 \text{ µm}$. This brings about the periodicity of $a = d + g$ in both $y$ and $z$ directions. The substrate that accommodates the KTP disks should be transparent in practice. Among a variety of available polymers, polymethylpentene, for example, can provide transparency as well as a low refractive index around 1.5 that is relatively independent of the wavelength in the THz range [39, 40]. Although patterning of a ferroelectric crystal is not as conventional as that of semiconductor, e.g. Si, the simplicity of our structure in microscale will allow the fabrication via mechanical dicing [41] or laser ablation [42].

3.1 Anisotropic transmission and reflection spectra of the KTP metasurface

Studying the uniformly distributed KTP disk array, we first calculate the anisotropic transmission and reflection spectra as a function of the diameter and the wavelength using the FDTD method. Figures 2(b) and 2(c) show the calculated transmission and reflection spectra, respectively, under the $\gamma$-polarized incident electric field. The white dashed lines in the figures follow the induced electric and magnetic dipole resonances to highlight their crossing in the spectral domain as we vary the diameter of the disks. Along the two separate resonances, transmission is observed to be suppressed with the corresponding enhancement in the reflection spectrum, whereas reflection vanishes at their intersection as the two modes oscillate in phase and spectrally overlap with each other, forming a so-called Huygens source.
This demonstrates the unidirectional emission, i.e. reflectionless or transmissionless, at the multipolar resonances that can be used for THz amplitude modulation. Under the $z$-polarized incident THz wave, as shown in Figs. 2(d) and 2(e), similar resonant properties are observed in the transmission and reflection spectra, respectively, together with the apparent red-shift of the resonances. In this case, however, simultaneous suppression appears in both transmission and reflection at the crossing of the electric and magnetic dipole resonances. This corresponds to a significant absorption over 80% (see Appendix B for more detail) due to the larger absorption cross-section along the $z$-axis of the KTP crystal.

3.2 Electromagnetic functional responses of the KTP metasurface

Secondly, we calculate the effective permittivity and permeability of our proposed KTP metasurface through the scattering parameters [37, 43, 44] that can be directly obtained from the previous transmission and reflection data (see Appendix C for more detail). The multipolar resonance makes our structure versatile in electromagnetic response that covers the four quadrants of permittivity and permeability [45] described in Fig. 3(a). The real part of the calculated effective permittivity and permeability along the $y$-axis are shown in Figs. 3(b) and 3(c), respectively, where the excitation of the electric and magnetic resonances can be clearly located.

Based on the effective permittivity and permeability, one can now articulate the various functional responses of the proposed KTP metasurface. For example, near the crossing of the two dipole resonances, our KTP metasurface becomes a negative index material ($\varepsilon_{\text{eff},y} < 0, \mu_{\text{eff},y} < 0$). Along the separate dipole resonances, on the other hand, the KTP metasurface resembles a magnetic mirror ($\varepsilon_{\text{eff},y} > 0, \mu_{\text{eff},y} < 0$) at the magnetic dipole resonance and an electric mirror ($\varepsilon_{\text{eff},y} < 0, \mu_{\text{eff},y} > 0$) at the electric dipole resonance. Moreover, this metasurface displays versatility even at certain off-resonant regions, forming a near-zero index material ($\varepsilon_{\text{eff},y} \approx 0, \mu_{\text{eff},y} \approx 0$) or a transparent film ($\mu_{\text{eff},y} \approx \mu_0\varepsilon_0$). These
multifunctional behaviors under the \( y \)-polarization are summarized in Fig. 3(d), where each functional zone is marked with the corresponding quadrant in Fig. 3(a). Similarly, the real part of the effective permittivity and permeability are calculated for the polarization along the \( z \)-axis in Figs. 3(e) and 3(f), respectively, while their various functional behaviors are marked in Fig. 3(g).

4. Enhanced birefringence in the KTP metasurface

In comparison to Figs. 3(b)-3(d), the distribution of the effective parameters over the spectral domain and their functional behaviors in Figs. 3(e)-3(g) may seem to stay similar under the different polarization. However, the calculated birefringence defined by \( \Delta n = n_{\epsilon, \text{eff}} - n_{\mu, \text{eff}} \)
reveals that our metasurface can significantly enhance the intrinsic anisotropy that is present in bulk KTP.

**Figure 4.** (a) Enhanced birefringence in the KTP metasurface as a function of the disk diameter and the wavelength. (b) Transmission switching contrast of the KTP metasurface, defined by $10 \log(T_y/T_z)$, between the two orthogonal polarizations. The inset in (b) corresponds to the transmission switching contrast of a thin KTP film with the same thickness of 60 μm. (c) An example of switching functionality at the disk diameter of 180 μm, where the metasurface is a transparent film under y-polarized illumination and transforms into a magnetic mirror under z-polarized illumination near 410 μm in the spectrum. (d) The calculated transmission spectra corresponding to the effective parameters described in (c). (e) Another example of switching functionality at the disk diameter of 165 μm, where the metasurface is a magnetic mirror under z-polarized illumination while it becomes an electric mirror under y-polarized illumination near the wavelength of 400 μm. (f) The calculated transmission spectrum corresponding to the effective parameters described in (c).

Figure 4(a) shows the effective birefringence, i.e. $\Delta n_{\text{eff}}$, which is calculated as a function of the disk diameter and the wavelength. In the FDTD calculation, the effective birefringence $\Delta n_{\text{eff}}$ is given by $\Delta n_{\text{eff}} = \left( \phi_{T,y} - \phi_{T,z} \right) \lambda / 2\pi h$, where $\phi_{T,y}$ and $\phi_{T,z}$ are the phase of the transmitted THz wave polarized along the y- and z-direction, respectively. In this case, the effective birefringence is sharply increased near the dipole resonances and can be tailored from −5 to 5, while the value in bulk KTP remains around 0.65. This leads to a high transmission switching contrast between the two orthogonal polarizations, defined by $10 \log(T_y/T_z)$, near the multipolar resonances, as shown in Fig. 4(b), where the extinction ratio can be up to 40 dB for a single layer of the KTP metasurface. In comparison, the transmission switching contrast of a 60 μm thin KTP film is also shown in the inset of Fig. 4(b), where the extinction ratio barely reaches 5 dB in this spectral region.

The enhanced anisotropy allows the designed metasurface to sharply switch its functional behavior when we change the polarization of the incident THz wave. Figure 4(c) describes an
example in which the calculated effective parameters are plotted for each polarization at the disk diameter of 180 μm. In this case, the system resembles a transparent film under γ-polarization with $T_\gamma > 80\%$, while it becomes a magnetic mirror under z-polarization near 410 μm in the spectrum. The corresponding transmission spectrum under each polarization is shown in Fig. 4(d) for comparison, where the transmission switching contrast reaches 20 dB. Another example is given in Fig. 4(e) at the disk diameter of 165 μm, where the metasurface is a magnetic mirror under z-polarization and transformed into an electric mirror under γ-polarization near the wavelength of 400 μm. Figure 4(f) shows the simultaneous suppression in their transmission spectra at the corresponding wavelength.

5. A gradient KTP metasurface for wavefront control

Finally, we consider a nonuniform distribution in the size of KTP disks to design an asymmetric interference pattern in the far-field. Imitating a phased array antenna for a wavefront manipulation, one may steer the THz beam by modulating the scattering phase at each disk in a fixed geometry. In order to study the phase change at each scatter center, we first calculate the transmission spectrum through a unit-cell that contains a single KTP disk on a substrate ($n = 1.5$). The unit cell in the FDTD simulation has a size of $a_y = 170$ μm and $a_z = 200$ μm with a periodic boundary condition, while the THz wave is normally incident on the KTP disk from the backside of the substrate.

Figures 5(a) and 5(b) show the transmission spectra under γ-polarization and the corresponding phase, respectively, as a function of the disk diameter. The change of the phase is very sensitive to that of the diameter near the crossing of the two resonances, which is utilized to tailor the far-field pattern with varied sizes of the disks. For example, a gradual 2π phase coverage is easily obtained when the diameter is changed from 20 μm to 120 μm, while a high transmission over 60% is well-maintained near the wavelength of 320 μm. In this range, denoted with the white arrow in Fig. 5(a), we propose a gradient KTP metasurface on a substrate that features a super-cell connecting four unit-cells along the z-direction with a different disk diameter in each.

Consequently, the interference between them results in deflection of the γ-polarized THz wave that is incident on the KTP disks from the backside of the substrate at a normal angle. Our FDTD calculation in Fig. 6(a) shows that the transmitted THz electric fields under γ-polarization propagates off-normal in the x-z plane. The deflection angle of 23° in the
simulation complies with the generalized Snell’s Law, \( \sin \theta = \lambda / (n \cdot L) \), where \( n \) denotes the refractive index of the background, i.e., air, and \( L = 4 \times a_z \) is the size of the super-cell. This provides the capability to engineer the deflection angle of the incident THz wave by manipulating the structure parameters \( L, N, a_z \) as well as the incident wavelength \( \lambda \).

As inherited from the intrinsic anisotropy in the \( x \)-cut KTP, the deflection property at the chirped KTP metasurface is naturally sensitive to the incident polarization, which makes it function as a polarizing beam-splitter. In contrast to the deflection under \( y \)-polarization, Fig. 6(b) shows that the transmitted THz electric fields under \( z \)-polarization propagates straight without any appreciable deflection. In this case, the designed metasurface resembles a Rochon prism, where the extraordinary ray is deflected while the ordinary ray passes through the prism undeviated.

Figure 6(c) shows the angular intensity distribution in the far-field for each polarization that is calculated using Fresnel–Kirchhoff integral. This far-field analysis confirms that more than 80% of THz transmission is deflected under \( y \)-polarization at the angle of 23° off-normal, while approximately 60% of the transmission under \( z \)-polarization passes without deflection. At the deflection angle of 23°, the switching contrast is calculated to be larger than 20:1.

6. Conclusion

In conclusion, we have demonstrated the anisotropic multipolar scattering in all-dielectric metasurfaces based on the ferroelectric crystal, KTP, for efficient manipulation of electromagnetic waves in the THz spectral region (0.6 – 1.5 THz). While we adjust the aspect ratio of the KTP disks, various electromagnetic responses have been articulated in terms of the effective permittivity and permeability of the designed metasurface. The intrinsic anisotropy in the \( x \)-cut KTP was significantly enhanced near the multipolar resonances, which allows a sharp switching of its functional behavior with the contrast that reaches 40 dB for a single layer (60 \( \mu \)m) of the KTP metasurface. The anisotropic scheme of the multipolar scattering was also implemented in a chirped KTP metasurface that can be used as a subwavelength-thin polarizing beam-splitter for THz waves.

Our study in this paper facilitates an efficient manipulation of THz waves in various ferroelectrics that would provide different semi-transparent spectral regions, showing high potential for a monolithic integration of the generation and the manipulation of THz waves in ferroelectric crystals.
Appendix A: Absorption coefficient and refractive index of KTiOPO₄ crystal in the terahertz region at room temperature (296 K)

The optical properties along the crystal axes of KTiOPO₄ (KTP) in the terahertz (THz) region at room temperature [28] are shown in Fig. 7. As shown in Fig. 7(a), the KTP crystal exhibits high refractive indices and a strong birefringence ($\Delta n = n_x - n_y \approx 0.65$), which do not appreciably change in the frequency range of 0.3 THz - 1.5 THz at room temperature. In this range, the absorption coefficients of $\alpha_x \approx \alpha_y < 15 \text{ cm}^{-1}$, $\alpha_z < 50 \text{ cm}^{-1}$ are also well-maintained, as depicted in Fig. 7(b). If we utilize this spectral window below 1.5 THz to avoid the strongest phonon lines, the absorption in KTP can, in fact, be comparable to that of Si near the band-edge at room temperature [14, 15, 19].

![Fig. 7. (a) Refractive indices and (b) absorption coefficient of KTiOPO₄ crystal in the terahertz region (0.3 THz – 1.5 THz) at room temperature (296 K) [28].](image)

Appendix B: Absorption in the uniform KTiOPO₄ metasurface

Studying the uniformly distributed KTP disk array, we calculate the anisotropic absorption spectra as a function of the diameter and the wavelength using the FDTD method. Figs. 8(a) and 8(b) show the calculated absorption spectra under the $y$-polarized and $z$-polarized incident electric field, respectively. The white dashed lines in the figures follow the induced electric and magnetic dipole resonances to highlight their crossing in the spectral domain as we vary the diameter of the disks. A significant enhancement of absorption is observed at the crossing of the resonances for both polarizations. In the case of a $z$-polarized incident electric field, the absorption can be as large as 80% at the crossing.

![Fig. 8. Calculated absorption of the square arrays of KTP disk metasurface with $h = 60 \mu$m, and $a = d + g$, where $g = 60 \mu$m under (a) $y$-polarized and (b) $z$-polarized illuminations. The diameter $d$ is varied from 60 µm to 200 µm. The white dashed lines follow the induced](image)
magnetic (MD) and electric (ED) dipole resonances, and highlight their crossings in the spectral domain as we vary the disk diameter.

Appendix C: Determination of the effective parameters for the metasurface on a substrate

First, the total scattering parameters (S parameters), which relates the incoming waves to the outgoing waves at the top and the bottom of the metasurface, can be directly obtained from the FDTD simulation. This is followed by the transfer matrix $M$ of the overall system, which can be derived from the $S$ parameters as follows,

$$
S = \begin{pmatrix}
S_{11} & S_{21} \\
S_{12} & S_{22}
\end{pmatrix}, 
M = \begin{pmatrix}
S_{21} - S_{11} \cdot S_{22} / S_{12} & S_{22} / S_{12} \\
-S_{11} / S_{12} & 1 / S_{12}
\end{pmatrix}
$$

(5)

Here, we treat the overall structure as a two-layer system that is separated by zero-thickness vacuum. In this case, $M$ can then be decomposed into the product of the transfer matrices of each layer [43],

$$
M = M_{\text{substrate}} \cdot M_{\text{metasurface}}
$$

(6)

Since the substrate is set to be an infinitely thick medium in the simulation, it is simply described by the boundary matrix, i.e. the transfer matrix across the interface from the free space into the substrate,

$$
M_{\text{substrate}} = \begin{pmatrix}
1 + z_b & 1 - z_b \\
2 & 2 \\
1 - z_b & 1 + z_b \\
2 & 2
\end{pmatrix}
$$

(7)

where $z_b$ is the impedance of the substrate. Substituting $M_{\text{substrate}}$ into Eq. (6), the effective transfer matrix of the metasurface in vacuum becomes,

$$
M_{\text{metasurface}} = M_{\text{substrate}}^{-1} \cdot M
$$

(8)

From the calculated $M_{\text{metasurface}}$, effective $S$ parameters of the free standing metasurface $S_m = \begin{pmatrix}
S_{11_m} & S_{21_m} \\
S_{12_m} & S_{22_m}
\end{pmatrix}$ can be derived according to Eq. (5). However, due to the presence of the substrate, $S_{11_m}$ is no longer equal to $S_{22_m}$. Note that this asymmetric response is not the intrinsic property of the induced multipole resonances. Therefore, for such an inhomogeneous metamaterial, if the asymmetric response is small enough, the effective refractive index and the impedance can still be calculated as follows [43,44],

$$
n = \pm \cos^{-1} \left( \frac{1}{2 S_{21_m}} \left[ 1 - \left( S_{11_m} \cdot S_{22_m} - S_{21_m^2} \right) \right] \right) + \frac{2 \pi l}{k_0 h}
$$

(11)

$$
z = \pm \sqrt{ \frac{(1 + S_{11_m})(1 + S_{22_m}) - S_{21_m^2}}{(1 - S_{11_m})(1 - S_{22_m}) - S_{21_m^2}} }
$$

(12)

where $l$ is an integer, and we take $\text{Im}(n) \geq 0$ and $\text{real}(z) \geq 0$. The calculated $n$ and $z$ under $y$-polarized and $z$-polarized illuminations are shown in Fig. 9. Based on the effective refractive index and the impedance above, the effective permittivity and permeability can be readily calculated as $\varepsilon = n / z$ and $\mu = n z$. 
Fig. 9. Retrieved effective refractive indices of the metasurface on the substrate under (a) \( y \)-polarized illumination and (b) \( z \)-polarized illumination. Retrieved effective impedance of the metasurface on the substrate in log scale under (c) \( y \)-polarized illumination and (d) \( z \)-polarized illumination.

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