

State Switching of Terahertz Reflection and Orbital Angular Momentum in Phase Change Metasurfaces

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Abstract—Metasurfaces with dynamically switchable functions have received extensive attention, and are in high demand in various applications. In this work, dynamically switchable metasurfaces are proposed based on phase change material—vanadium dioxide. They consist of vanadium dioxide blocks, silicon dioxide spacer, and gold film. By changing the size of vanadium dioxide block, vanadium dioxide in the metallic state forms a gradient metasurface. A specially arranged gradient metasurface is designed to achieve a 360° phase modulation capability. Normally incident plane wave is reflected to the right side at the angle of 36.9° at 2.5 THz. When vanadium dioxide switches from the metallic state to the insulating state, the switching of anomalous reflection and specular reflection is realized. In addition, when vanadium dioxide is metal, a vortex beam generator is implemented to generate orbital angular momentum beams with $l = 1$ and $l = 2$. The number of orbital angular momentum mode can be switched from $l = 0$ to $l = 1$ or $l = 2$ by changing the state of vanadium dioxide. Since the structure of meta-atom is a square block, the design is simple and easy to integrate. At the same time, the switchable function is accurately implemented without side lobe. The proposed design has potential applications in terahertz switching and communication.

Index Terms—Metasurface, vanadium dioxide, anomalous reflection, orbital angular momentum.

I. INTRODUCTION

ACHIEVING full control on electromagnetic wave is greatly significant. It has urgent needs in the fields of communication, energy, national defense, and so on. However, the ability of traditional natural materials to control electromagnetic wave is limited, which hinders the development of electromagnetic device. Metamaterials are specially designed subwavelength microstructures. According to requirements, artificial meta-atoms are designed and then combined in a special arrangement. Metamaterials are used to build devices that effectively control amplitude, phase, polarization, and wavefront of electromagnetic wave. Therefore, metamaterials have received extensive attention from scientific and engineering communities for their unprecedented control over electromagnetic wave at the subwavelength scale. By appropriately controlling the properties

of electromagnetic wave, many novel physical phenomena and interesting applications are obtained. Examples include negative refraction [1]–[3], invisible cloak [4]–[6], and perfect lens [7]–[9].

Recently, metasurfaces have become a hot topic of research. They are two-dimensional metamaterials that combine artificial electromagnetic microstructures in spatial order. Metasurfaces, as a planar version of metamaterials, have realized many new phenomena of electromagnetic wave regulation that cannot be achieved by three-dimensional bulk metamaterials. It uses the abrupt effect on the interface to achieve the control of electromagnetic wave. This improves efficiency and reduces loss of electromagnetic wave. Metasurfaces are simple to fabricate, easy to integrate, and provide solutions for on-chip applications. Gradient metasurfaces are formed by gradient phase distribution. Some applications of gradient metasurfaces are proposed. In 2016, N. M. Estakhri *et al.* investigated theoretical limitations and potentials of passive gradient metasurfaces to manipulate arbitrary wave [10]. Unlike similar metasurfaces using traditional ray-optics method, the extreme-angle wave-bending metasurface they employed significantly improved the overall efficiency by 30%. In 2017, Y. Li *et al.* carried out theoretical analysis and experimentally verified asymmetric wave transmission in lossy acoustic gradient-index metasurface [11]. In 2018, J. Li *et al.* designed three refractive metasurfaces. These metasurfaces are capable of anomalous reflection, redirecting normally incident plane waves to 60° , 70° , and 80° on transmission [12]. The efficiency of the bianisotropic design exceeds 90%, while the corresponding generalized Snell's law based design is well below this value. In 2020, H. Kazemi *et al.* introduced a chiral gradient metasurface to achieve redirection of transmission and perfectly rotate the polarization of the refracted wave [13]. Their results showed that plane wave at normal incidence is deflected by 45° as a refracted plane wave with a power efficiency of 72%, accompanied by a 90° polarization rotation. In addition, vortex beam carrying orbital angular momentum (OAM) can be generated by spiral phase distribution. In 2016, D. Hakobyan *et al.* reported on the fabrication and characterization of optical vortex generators made of metallic metasurfaces [14]. In 2018, Y. Shen *et al.* presented a metasurface-based reflective-type approach to form a nondiffractive Bessel beam carrying OAM [15]. The prototype integrated the planar feeding source with the metasurface. In 2019, M. R. Akram *et al.* designed a novel bilayer meta-atom with a periodic unit cell-based transmission efficiency of up to 85% [16]. These meta-atoms were then used to construct metasurfaces that generate vortex beams carrying

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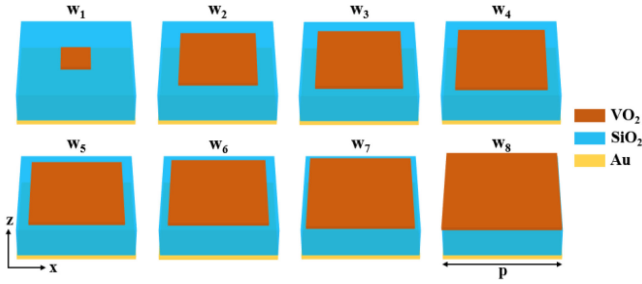


Fig. 1. 3D schematic diagram of the designed eight different meta-atoms. The dimensions are $w_1 = 6.5 \mu\text{m}$, $w_2 = 16.8 \mu\text{m}$, $w_3 = 18.5 \mu\text{m}$, $w_4 = 19.4 \mu\text{m}$, $w_5 = 20.2 \mu\text{m}$, $w_6 = 21.2 \mu\text{m}$, $w_7 = 22.8 \mu\text{m}$, and $w_8 = 25 \mu\text{m}$.

OAM. In 2020, B. Liu *et al.* proposed a concept of multifunctional vortex beam [17]. It is realized by a dynamic reflective metasurface which is capable of controlling vortex beam spatiotemporally.

Vanadium dioxide (VO_2) is an excellent tunable material. It has special phase transition properties. VO_2 is an insulator with a monoclinic crystal structure at room temperature. Once phase transition temperature is exceeded, VO_2 changes into tetragonal rutile crystal and acts as a metal. This insulator-to-metal transition is fastly achieved by applying thermal, electrical, or optical stimulus. This structural transition leads to significant changes in electrical and optical properties of VO_2 . The conductivity of VO_2 increases by several orders of magnitude during the transition. Up to now, research on VO_2 -based devices has involved many aspects, such as optical switch [18]–[20], absorber [21]–[23], and filter [24]–[26]. In 2018, M. Sun *et al.* proposed a photonic switch based on VO_2 material, whose structure is composed of an array of hexagonal nanoholes [27]. It achieves a maximum transmission rate of 37% at optical communication band. In 2020, M. Zhang *et al.* designed a terahertz absorber composed of a graphene-spacer- VO_2 -spacer-metal structure with narrowband and broadband properties [28]. A band of 100% absorption is reached at 1.37 THz. In the frequency range of 1.05–2.35 THz, broadband absorption is formed with absorption >90%. In 2021, Z. Che *et al.* presented a controllable terahertz filter with dual narrowband characteristics, and its structure consists of two n-shaped waveguides and one VO_2 defect [29]. Switching between passband and stopband is achieved at 1.287 THz and 1.447 THz. The proposed filter has great application prospects in the field of temperature-controlled switches in integrated photonic circuits.

In this work, switchable metasurfaces are designed by exploiting the special properties of phase change material VO_2 . By arranging VO_2 blocks with different sizes, eight meta-atoms are designed. When VO_2 is in the metallic state, the metasurface formed by eight meta-atoms achieves phase coverage of 0–360°. Dynamically switchable gradient metasurface and vortex beam generator are presented. At the frequency of 2.5 THz, plane wave under normal incidence is anomalously reflected at 36.9°, and this behavior is independent of polarization. The designed vortex beam generators generate OAM beams with $l = 1$ and $l = 2$. When VO_2 changes from the metallic state to the insulating state, anomalous reflection switches to specular reflection. And

the beam generated by vortex beam generator switches from $l = 1$ or $l = 2$ to $l = 0$. Different from circularly polarized wavefront control [30], this work is mainly applied to wavefront control on linearly polarized wave. Although many works on gradient metasurface have been proposed [31], there are still few studies on VO_2 -based reconfigurable metasurface. Compared with [32], our design achieves phase coverage of 360° with phase difference 45° between adjacent meta-atoms, and realizes the desired function without side lobe.

II. DESIGN AND METHOD

Three-dimensional schematic diagram of the designed switchable meta-atoms is shown in Fig. 1. The designed metasurfaces consist of eight meta-atoms with different VO_2 block sizes. Each meta-atom is composed of three parts: the top VO_2 block, the middle silicon dioxide spacer, and the bottom gold film. The period of meta-atom is $P = 25 \mu\text{m}$. The thicknesses of VO_2 blocks, silicon dioxide spacer, and gold film are $1 \mu\text{m}$, $6 \mu\text{m}$, and $1 \mu\text{m}$, respectively. The dimension of VO_2 blocks changes from w_1 to w_8 . Electromagnetic simulation of the proposed switchable metasurface is carried out with the help of finite element method (commercial software-Comsol Multiphysics). Periodic boundary conditions are used for calculating unit cell along x and y directions, and linear plane wave shines structure from z direction. Adaptive mesh refinement is adopted, which helps to ensure the convergence of the simulated results. Silicon dioxide acts as a dielectric layer with relative dielectric permittivity of 3.85 [33], [34]. The bottom gold film is assumed as a lossy metal with the conductivity of $4.561 \times 10^7 \text{ S/m}$. Dielectric permittivity of VO_2 in the terahertz range is described by Drude model $\varepsilon(\omega) = \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\omega\gamma}$ [35]–[37]. In the above equation, $\varepsilon_\infty = 12$ is dielectric permittivity at the infinite frequency, ω_p is plasma frequency dependent on conductivity, and $\gamma = 5.75 \times 10^{13} \text{ s}^{-1}$ is collision frequency. When VO_2 is in the metallic (insulating) state, the conductivity is $2 \times 10^5 \text{ S/m}$ (200 S/m) and its ω_p is $1.143 \times 10^{15} \text{ rad/s}$ ($3.6149 \times 10^{13} \text{ rad/s}$). Phase transition process of VO_2 is stimulated by optical pumping [38], [39].

III. RESULTS AND DISCUSSIONS

The overall functional behavior of metasurface arises from the superposition of wavefronts of different meta-atoms. Therefore, ensuring 360° phase coverage is a key point in the design. Reflection coefficient should also be maintained at a certain level to ensure efficiency. To achieve arbitrary manipulation of the reflected wavefront, eight different meta-atoms are designed. In simulation, the reference plane is set on the top of VO_2 block. Simulated results are shown in Fig. 2. When VO_2 is in the metallic state, phase range increases from -135° to 180° as the size of VO_2 block changes. At the target frequency of 2.5 THz, the designed eight meta-atoms achieve phase coverage of 0–360°, and phase difference between two adjacent cells is stable around 45°. Reflection amplitude of eight meta-atoms remains above 0.65, which ensures a certain reflection efficiency. This result verifies that reflection phase is effectively modulated

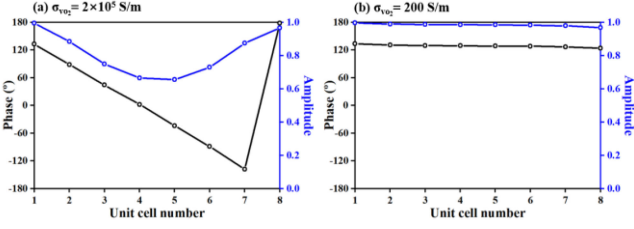


Fig. 2. Reflection phases (black) and amplitudes (blue) of eight meta-atoms with y-polarized wave under normal incidence for $\sigma_{VO_2} = 2 \times 10^5$ S/m (a) and $\sigma_{VO_2} = 200$ S/m (b) at 2.5 THz.

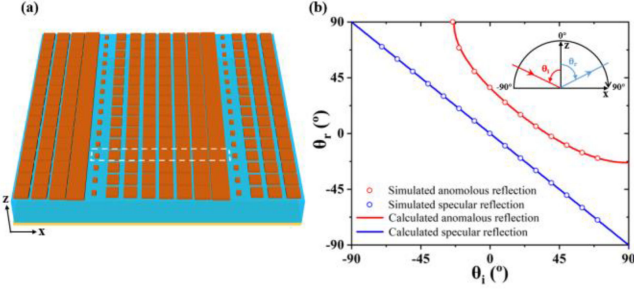


Fig. 3. (a) Structural diagram of the designed gradient metasurface. Gradient metasurface has different beam steering functions under different VO_2 states. (b) Simulated and calculated results of reflection angles with different incident angles in two states.

by changing VO_2 block size. However, when VO_2 is in the insulating state, no matter how to change the size of VO_2 block, it has little effect on the fluctuation of phase and amplitude. It is the characteristic of VO_2 , a phase change material, that enables the realization of switchable metasurface.

A. Gradient Metasurface

As shown in Fig. 3(a), eight meta-atoms are combined along the x-axis in order of decreasing phase to form a supercell. To simulate deflection effect, eight supercells are set along x direction, and periodic boundary conditions are set along y direction. Electromagnetic wave is incident at different angles relative to z axis. According to the generalized Snell's law, metasurface with a certain phase gradient can be formed by an array of scatterers with subwavelength spacing. The designed gradient metasurface theoretically creates an additional wave vector and changes the wavefront of the reflected beam. The structure of meta-atom is square, thus enabling beam steering. In the defined coordinate system (the inset in Fig. 3(b)), reflection angle θ_r is derived as $\theta_r = \sin^{-1}(-\sin \theta_i + \xi/k_0)$, where θ_i is incident angle, $\xi = \frac{2\pi}{SP}$ is the gradient value, and $k_0 = \frac{2\pi}{\lambda}$ is the wavevector at wavelength λ [40]. Therefore, by theoretical calculation, two results are obtained. When phase gradient is zero, the calculation shows $\theta_r = -\theta_i$, which is the phenomenon of specular reflection (blue curve in Fig. 3(b)). When VO_2 switches from the insulating state to the metallic state, phase gradient is formed. The relationship between θ_r and θ_i is obtained by substituting period P and wavelength λ corresponding to 2.5 THz into the above formula. The calculated result of anomalous reflection is shown in the red curve in Fig. 3(b). In order to verify the reliability of the switchable function of anomalous reflection and specular reflection, a series of incident angles are selected for

simulation. Simulated results are shown in Fig. 3(b), red circles and blue circles represent the relationship between θ_r and θ_i of anomalous reflection and specular reflection, respectively. Obviously, simulated results are in good agreement with calculated curves. It is demonstrated that the designed gradient metasurface can dynamically switch between two functions of anomalous reflection and specular reflection. In addition, there is a critical angle $\theta_{ic} = \sin^{-1}(-\sin 90^\circ + \xi/k_0)$ for θ_i such that as $|\theta_i| > |\theta_{ic}|$, the reflected beam becomes a surface wave bounded on the metasurface which cannot radiate to free space [41].

In the above results, three special incident angles are selected for analysis in the far-field scattering patterns. As shown in Fig. 4, far-field scattering patterns of the reflected beams in different VO_2 states exhibit different phenomena at the incident angles of 0° , 17.5° , and 36.9° . In Fig. 4(a), when plane wave is incident vertically ($\theta_i = 0^\circ$), it is anomalously reflected at reflection angle $\theta_r = 36.9^\circ$. When VO_2 switches to the insulating state, the reflected beam in Fig. 4(d) is reflected out in the form of specular reflection with $\theta_r = 0^\circ$. The anomalously reflected beam has no other high-intensity side lobes, and the intensity reaches more than half of the specularly reflected beam. Through calculation in Fig. 4(b), we get the special negative reflection phenomenon of $\theta_r = \theta_i$ when $\theta_i = 17.5^\circ$. The obliquely incident beam returns along the original path. And it is switched to positive reflection ($\theta_r = -17.5^\circ$) in Fig. 4(e). In Fig. 4(c), when $\theta_i = 36.9^\circ$, the anomalously reflected beam is perpendicular to the metasurface ($\theta_r = 0^\circ$). The result in Fig. 4(f) is still in the form of specular reflection.

B. Vortex Beam Generator

In 1992, L. Allen *et al.* firstly confirmed that a light beam can carry OAM [42]. The realization of vortex beam carrying OAM through metasurface has become a research hotspot. OAM waves have applications in optical, terahertz, and microwave regions. Among them, the use of OAM in wireless communication to improve channel capacity has great application value [43]. Phase distribution of OAM wave is described by $e^{il\theta}$, where l is OAM mode number and θ is azimuth angle. The well-known spin angular momentum (SAM) has a fixed state with linear and circular polarizations of $s = 0$ and $s = \pm 1$, respectively. OAM provides an infinite number of orthogonal states. OAM mode number can be $l = 0, \pm 1, \pm 2, \pm 3, \dots$, where wavefront phase of $l = 0$ vortex beam is uniform. When l is a non-zero integer, vortex beam has a spiral phase distribution.

To realize vortex beam generator producing OAM wave, two metasurfaces composed of eight meta-atoms are designed in Fig. 5. Space and reflection phase are discretized, and the metasurfaces with 48×48 meta-atoms are divided into distinct regions. Perfect matched layers are set along x and y directions. Phase difference of each region is 45° . For $l = 1$, the metasurface is divided into eight regions, and for $l = 2$, the metasurface is divided into sixteen regions. Eight kinds of meta-atoms are arranged in the corresponding area in the xoy plane, and plane wave is incident on the metasurface along z direction for simulation and observation.

Simulated results of far-field scattering patterns are shown in Fig. 6 ($l = 1$) and Fig. 7 ($l = 2$). The results show that

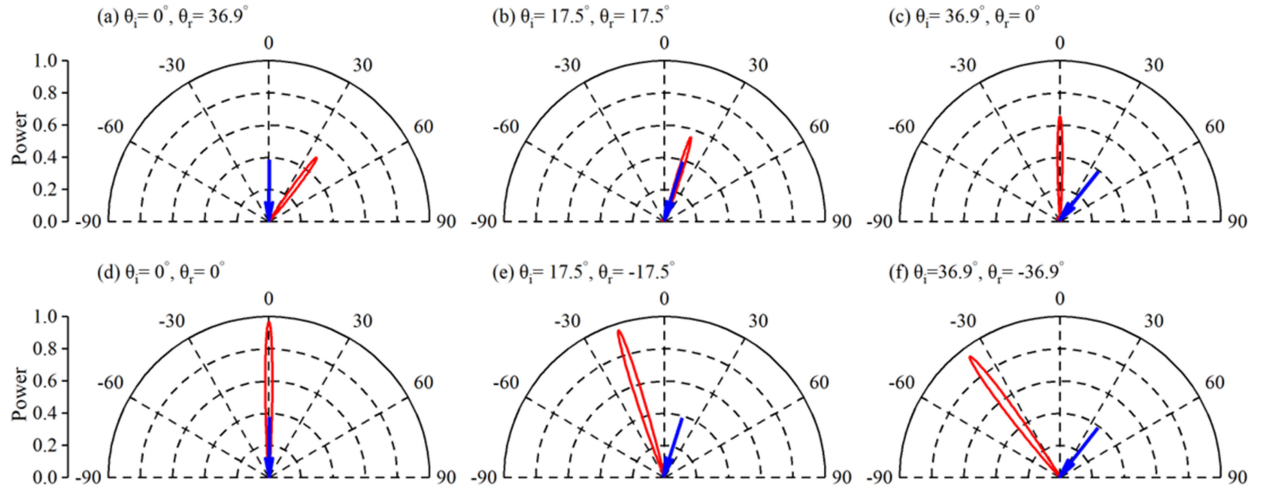


Fig. 4. Simulated deflection angle and power of the reflected beam (red curve) at 2.5 THz. Incident wave is polarized along y direction. Blue arrows only indicate the direction of incidence. (a)–(c) are far-field scattering patterns with $\sigma_{\text{VO}_2} = 2 \times 10^5 \text{ S/m}$. (d)–(f) are far-field scattering patterns with $\sigma_{\text{VO}_2} = 200 \text{ S/m}$.

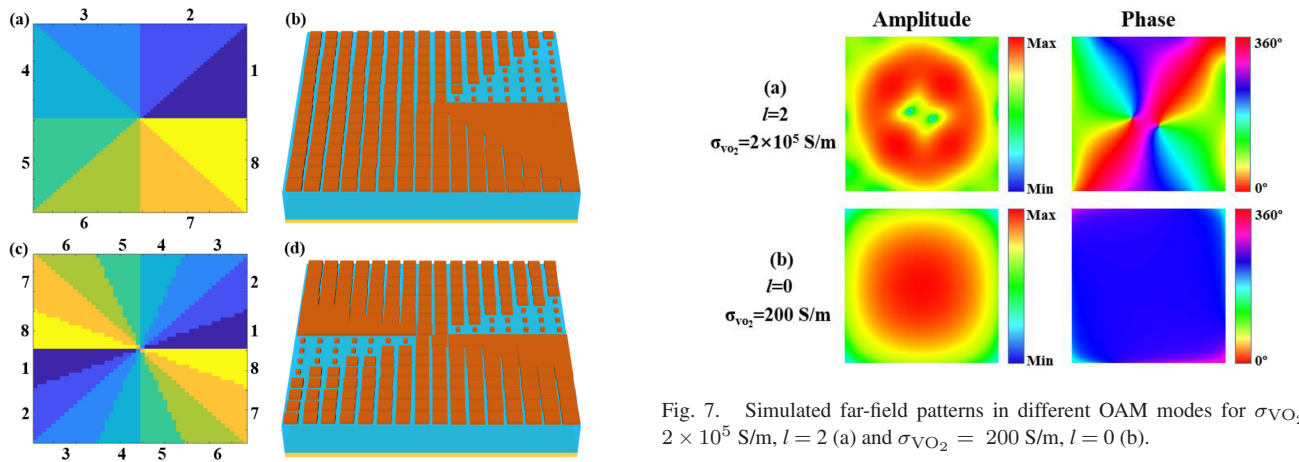


Fig. 5. Spatial distribution of the proposed metasurface consisting of eight regions 1–8 representing by different colors in (a) $l = 1$ and (c) $l = 2$. Part of the simulated metasurface for generating OAM $l = 1$ (b) and $l = 2$ (d).

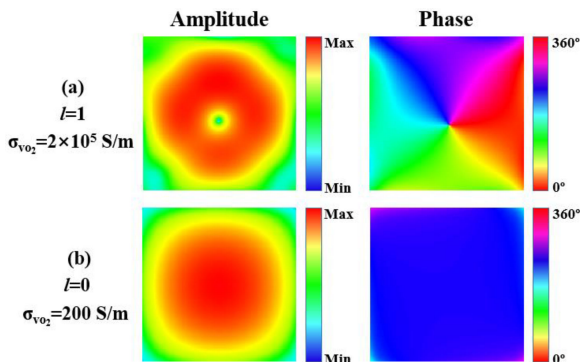


Fig. 6. Simulated far-field patterns in different OAM modes for $\sigma_{\text{VO}_2} = 2 \times 10^5 \text{ S/m}$, $l = 1$ (a) and $\sigma_{\text{VO}_2} = 200 \text{ S/m}$, $l = 0$ (b).

when $\sigma_{\text{VO}_2} = 2 \times 10^5 \text{ S/m}$, the designed metasurface forms a vortex beam carrying OAM. Amplitude of OAM is a ring-shaped intensity distribution with a deep null region at the center. For $l = 2$, the central area is split into two null points. Neither amplitude

Fig. 7. Simulated far-field patterns in different OAM modes for $\sigma_{\text{VO}_2} = 2 \times 10^5 \text{ S/m}$, $l = 2$ (a) and $\sigma_{\text{VO}_2} = 200 \text{ S/m}$, $l = 0$ (b).

of $l = 1$ nor amplitude of $l = 2$ are completely uniform. This is due to the finite size of the metasurface and the discrete phase distribution in vortex generator. Phase results of OAM show a 360° phase rotation for $l = 1$ in Fig. 6(a) and a 720° phase rotation for $l = 2$ in Fig. 7(a). The generation of OAM with modes $l = 1$ and $l = 2$ is confirmed from both amplitude and phase profiles. When $\sigma_{\text{VO}_2} = 200 \text{ S/m}$, the generated beams are plane wave with $l = 0$ in Fig. 6(b) and Fig. 7(b), and its amplitude and phase distributions are completely uniform. The results in Fig. 6 and Fig. 7 show that vortex beam generator realizes the switching of OAM mode from $l = 1$ and $l = 2$ to $l = 0$. Phase change of VO_2 disrupts the spiral phase distribution of meta-atoms. Consequently, the wavefront of OAM generator is reconstructed.

IV. CONCLUSION

To summarize, switchable metasurfaces are proposed, and they are capable of anomalous reflection and generation of OAM. By changing the size of VO_2 block, eight meta-atoms are designed to achieve a phase range coverage of $0\text{--}360^\circ$. Using the proposed meta-atoms through appropriate arrangement, gradient metasurface and vortex beam generator are designed.

The designed gradient metasurface achieves dynamic switching between anomalous reflection and specular reflection at the frequency of 2.5 THz. When $\sigma_{\text{VO}_2} = 2 \times 10^5 \text{ S/m}$, the proposed vortex beam generator excites terahertz wave carrying OAM modes $l = 1$ and $l = 2$. OAM mode can be switched from $l = 1$ or $l = 2$ to $l = 0$ by changing the state of VO_2 . Simulated results clearly tell that precise control of terahertz wavefront is realized for linearly polarized wave. Due to the characteristics of simple structure design and easy integration, the potential applications of the designed metasurfaces are anticipated for dynamic beam steering. Our work may pave new paths in dynamically switchable terahertz metasurfaces.

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