

Tunable oriented mid-infrared wave based on metasurface with phase change material of GST

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ABSTRACT

Dynamically controlling the mid-infrared electromagnetic waves with tunable metasurfaces remains a challenging task. Phase change material of Ge₂Sb₂Te₅ (GST) has shown tremendous advantages in constructing reconfigurable metasurface. In this work, we design a metasurface with GST to dynamically focus and deflect the beam at wavelength of 8.5 μm with a fixed structure. The designed metasurface is composed of GST nanocylinders on a Calcium Fluoride (CaF₂) substrate. The focusing and deflection characteristics are manipulated by artificially controlling the value of crystalline fraction of each GST cylinder. In addition, we studied the diffraction pattern at a distance of 2 m for oriented deflection and its broadband performance. This method improves the degree of freedom of active modulation and provides a new route for tunable optical communication devices.

Introduction

In the past decades, metamaterials and metasurfaces have attracted wide attention since they offer large degrees of freedom in engineering optical field, including its amplitude, phase and polarization [1–4]. Compared with 3D metamaterials, 2D metasurfaces have many distinct advantages in manipulating electromagnetic waves. Based on metasurfaces, various novel devices have been designed and applied for various practical applications, such as polarization conversion [5–7], generation of optical beams carrying orbital angular momentum [8–10], holograms with high resolution [11–13] and focusing metalens [14–17]. In particular, active metasurfaces, as a new branch of metasurfaces, are reconfigurable and/or tunable in real time, which are originated from their tunable optical characteristics through external control, and may serve as multifunctional optical devices [18–21].

At present, the incorporation of materials with tunable optical properties, such as graphene [22–25], semiconductors [26–28], and phase change materials, is an effective route to achieve active metasurfaces. Among these materials, Ge₂Sb₂Te₅ (GST) is of particular interest since it exhibits great physicochemical characterizations of quick response, good stability, large number of switching cycles, and significant refractive index contrast between amorphous and crystalline states

[29–32]. For these reasons, more and more researchers have tried to achieve tunable metasurfaces with GST. In 2016, Chu et al. have studied the GST metasurfaces to demonstrate reconfigurable meta-devices in near-infrared utilizing its tunable optical properties as it undergoes phase transition [33]. In 2019, Choi et al. have reported an active metasurface for wavefront switching that can operate at near-infrared region with bandwidth more than 500 nm [34]. In 2020, Tian et al. have demonstrated that the structured phase-change alloy GST can support a diverse set of multipolar Mie resonances with active tunability [35]. Nevertheless, a tunable metasurfaces with GST working in the mid-infrared region still remains an interesting task.

In this work, we designed tunable metasurfaces working at wavelength of 8.5 μm by using GST nanocylinders on CaF₂ substrate. As proof-of-concept, an example of active beam control device, we implement two functional active devices: tunable focusing metalens and oriented deflector. When the geometry parameters are fixed, the focus of metalens and the orientation of beams can be artificially engineered by controlling the value of crystalline fraction of each GST nanocylinder. The diffraction pattern at a distance of 2 m for oriented deflection and the broadband performance are investigated. The combination of phase change material of GST increase degrees of freedom for light manipulation, which is an essential step towards practical applications of

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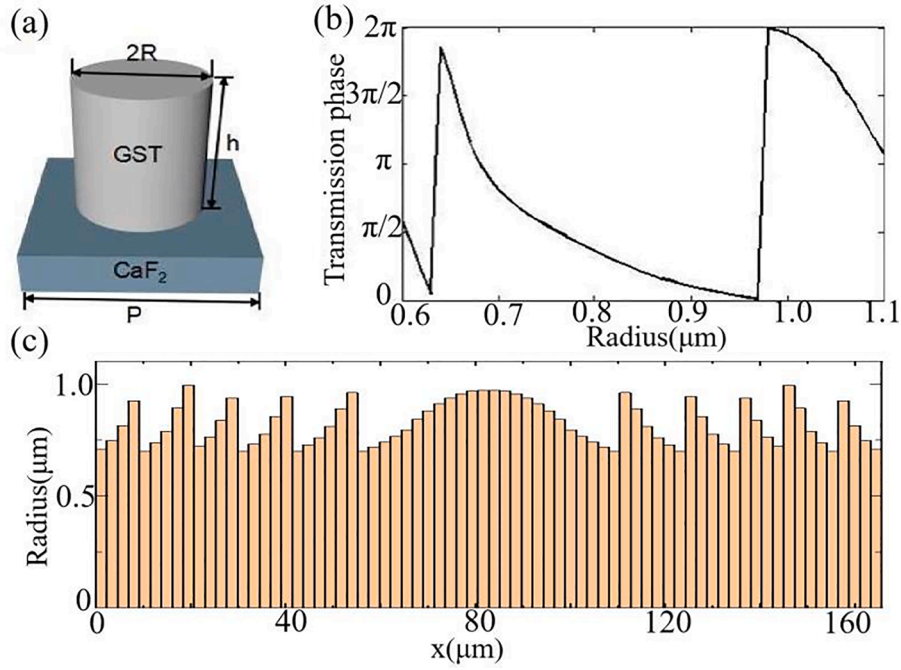


Fig. 1. (a) Unit-cell of the proposed structure. The geometrical parameters are set as: $p = 2.3 \mu\text{m}$, $h = 6.5 \mu\text{m}$. The radius of GST nanocylinder R varies with the position on metasurface. (b) Simulated transmission phase of unit-cell with the nanocylindrical radius varying from $R = 0.6 \mu\text{m}$ to $R = 1.1 \mu\text{m}$. (c) At the wavelength of $8.5 \mu\text{m}$, the required Radius distribution to focus x-polarized plane wave at a focal length of $42.5 \mu\text{m}$ when $m = 0.6$.

metasurfaces in the mid-infrared region. The proposed method can be widely used in mid-infrared communication scenarios, which not only facilitate integration and miniaturization, but also open up a new way for the design of optical communication devices in the future.

Results and discussions

Fig. 1(a) schematically shows the unit structure of our metasurface, where the periods in both x and y directions are $P = 2.3 \mu\text{m}$, the height of the GST nanocylinder is $h = 6.5 \mu\text{m}$. The radius of the GST nanocylinders varies with their position according to the requirement of designed functions. The material of substrate is chosen as CaF_2 due to its low absorption loss in mid-infrared frequency [36].

To numerically investigate the metasurfaces, a home-built program with finite-element method is implemented. An x-polarized light is normally incident on metasurfaces along the z direction. The periodical boundary conditions are used in both x and y directions, and perfectly matched layers are set in the z direction. The refractive index of GST can be tuned between $n = 3.98$ (amorphous phase) and $n = 5.8$ (crystalline phase) at wavelength of $8.5 \mu\text{m}$ [37]. For the intermediate state, its dielectric parameter can be predicted with the Lorentz-Lorentz relation [38]:

$$\frac{\epsilon_{\text{eff}}(\lambda) - 1}{\epsilon_{\text{eff}}(\lambda) + 2} = m \frac{\epsilon_{\text{cGST}}(\lambda) - 1}{\epsilon_{\text{cGST}}(\lambda) + 2} + (1 - m) \frac{\epsilon_{\text{aGST}}(\lambda) - 1}{\epsilon_{\text{aGST}}(\lambda) + 2} \quad (1)$$

where $\epsilon_{\text{cGST}}(\lambda)$ and $\epsilon_{\text{aGST}}(\lambda)$ are permittivity of GST as functions of working wavelength λ at the crystalline ($m = 0$) and amorphous states ($m = 1$), respectively. m represents the GST crystallization fraction, whose value ranges from 0 to 1. It is worth to note that a subtle change of volume of the GST pillars would happen during the phase transition [35]. Nevertheless, this effect is not under consideration in this work because it is not clear how such a volume change would impact the 3D GST pillars. In addition, such a subtle change would not significantly influence the spectral position or the strengths of the resonances and usually has not been taken into consideration in metasurface [39].

We start by investigating the optical response of GST nanocylinder.

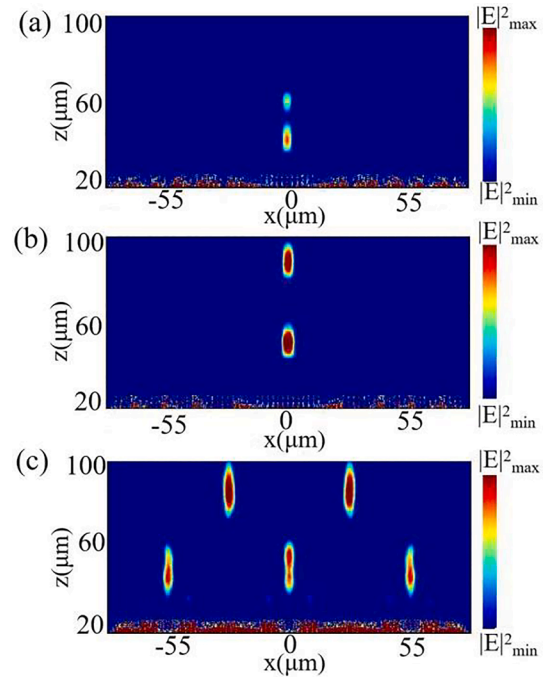


Fig. 2. Metasurface designed at wavelength of $8.5 \mu\text{m}$ with focal length of $f = 42.5 \mu\text{m}$ and GST crystallization fraction of $m = 0.6$. Simulated electric field intensity distribution in x - z plane for metalens with focus at (a) $(0, 42.5 \mu\text{m})$, (b) $(0, 42.5 \mu\text{m})$ and $(0, 68 \mu\text{m})$, (c) $(-55.2 \mu\text{m}, 42.5 \mu\text{m})$, $(-27.6 \mu\text{m}, 68 \mu\text{m})$, $(0 \mu\text{m}, 42.5 \mu\text{m})$, $(27.6 \mu\text{m}, 68 \mu\text{m})$ and $(55.2 \mu\text{m}, 42.5 \mu\text{m})$. The structure of metasurface keeps unchanged.

Fig. 1(b) shows the dependence of simulated phase of transmitted light on the value of the radius R . In this case, we fixed the GST crystallization fraction as $m = 0.6$. When the radius increases from $R = 0.6 \mu\text{m}$ to $R = 1.1 \mu\text{m}$, the phase of transmitted light varies over a full range of 0 to 2π . It

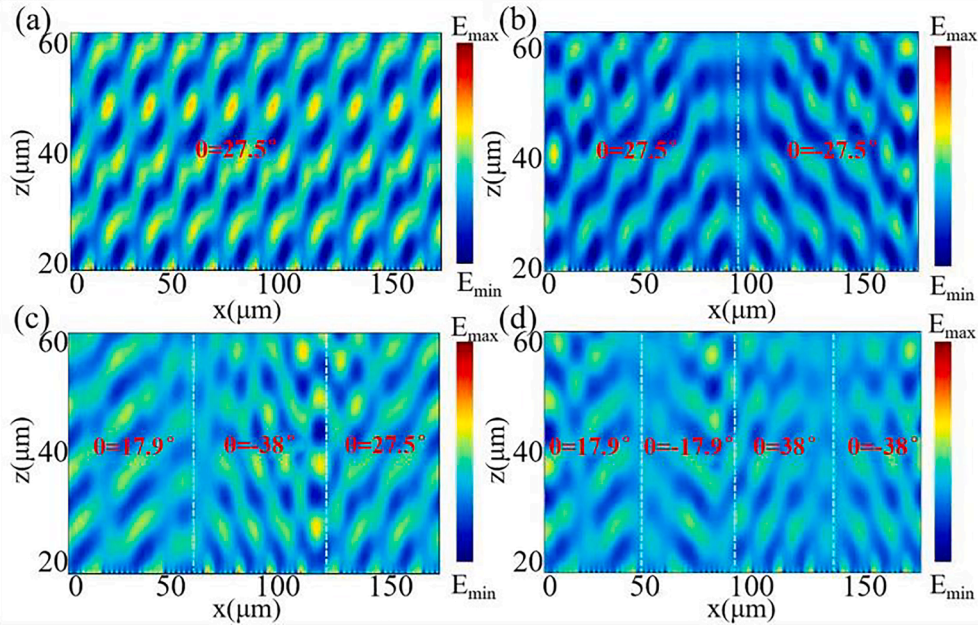


Fig. 3. Metasurface designed at wavelength of $8.5 \mu\text{m}$ with deflection angle of 27.5° and GST crystallization fraction of $m = 0.6$. Simulated electric field intensity distribution in x - z plane for deflectors with deflection beams of (a) single beam at angle of 27.5° , (b) two beams at angles of 27.5° and -27.5° , (c) three beams at angles of 17.9° , -38° , and 27.5° , (d) four beams at angles of 17.9° , -17.9° , 38° , and -38° . The structure of metasurface keeps unchanged.

indicates the great ability of GST nanocylinder to manipulate the transmission wavefront. In this work, we have not considered the coupling between neighboring structures for two reasons. First, the waveguide-like cavity resonances in nanopillars strongly concentrate the optical field inside the dielectric structures, resulting in the negligible interaction with the neighboring elements [40]. Second, we have considered the value of radius ranging from $0.6 \mu\text{m}$ to $1.1 \mu\text{m}$ and Fig. 1 (b) shows that most of them are smaller than half period, making the coupling effect negligible. Fig. 1(c) shows the required distribution of radius values of nanopillars on a focusing metalens, which could focus incident plane wave with wavelength of $8.5 \mu\text{m}$ at a distance of $42.5 \mu\text{m}$. The corresponding phase profile $\varphi(x)$ of the focusing metalens can be written as $\varphi(x) = -2\pi/\lambda \cdot \left(\sqrt{(x - x_0)^2 + f^2} - f \right)$, where λ is the incident wavelength, (x_0, f) represents the coordinate of an arbitrary focal point, and f is the pre-designed focal length. When the metasurface satisfies the phase distribution of $\varphi(x)$, a plane wave incident on the metasurface will be converged into a spherical wave. Combining Fig. 1(b) and (c), we can easily determine the radius of the GST nanocylinders on focusing metalens, which will be not shown in details due to the limitation of paper length. Note that, the number of GST nanocylinders is seventy-two.

Fig. 2(a) shows the simulated light intensity profiles of the designed focusing metalens at wavelength of $8.5 \mu\text{m}$ in x - z plane. As we mentioned before, the crystalline fraction of all GST nanocylinders are set as $m = 0.6$. It clearly illustrates that a strong focus forms at a distance of about $42.5 \mu\text{m}$ behind the metalens, which is in a good agreement with the designed value. Owing to the tunable optical response of GST nanocylinders, it is tried to achieve more focuses behind the metalens by individually manipulating the crystalline fraction of each unit element. To demonstrate, two different focusing functions are obtained by using the designed metasurface: two focuses at positions of $(0, 42.5 \mu\text{m})$ and $(0, 68 \mu\text{m})$, and five focuses at positions of $(-55.2 \mu\text{m}, 42.5 \mu\text{m})$, $(-27.6 \mu\text{m}, 68 \mu\text{m})$, $(0, 42.5 \mu\text{m})$, $(27.6 \mu\text{m}, 68 \mu\text{m})$ and $(55.2 \mu\text{m}, 42.5 \mu\text{m})$. In these processes, the structure of metasurface keeps unchanged. Fig. 2 (b) shows the simulated electric field intensity distribution of the metalens with two focuses in x - z plane, and the positions of simulated focuses are read as $(0, 42.5 \mu\text{m})$ and $(0, 68 \mu\text{m})$. Fig. 2(c) plots the

calculated electric field intensity distribution of the metalens with five focuses in x - z plane, and the positions of calculated focuses are $(-55.2 \mu\text{m}, 42.5 \mu\text{m})$, $(-27.6 \mu\text{m}, 68 \mu\text{m})$, $(0, 42.5 \mu\text{m})$, $(27.6 \mu\text{m}, 68 \mu\text{m})$ and $(55.2 \mu\text{m}, 42.5 \mu\text{m})$. The simulation results of the latter two cases are also in good agreements with the designed values.

The above investigations show that this reconfigurable metasurface with GST can be utilized to achieve function of oriented focusing. That is focusing the incident light to arbitrary positions by optimizing the GST crystalline fraction of each unit cell without changing the geometry. It could be attributed to the difference in optical response between GST unit elements with different crystallization rates. Therefore, the active GST metalens can be achieved by changing the environmental temperature or by external femtosecond laser pulse stimulus [41].

In addition, we designed tunable deflector using metasurface with GST nanocylinders to direct the incident light to different angles at the wavelength of $8.5 \mu\text{m}$. At first, a metasurface is designed with a single deflected beam at angle of 27.5° and the crystallization fraction of all GST nanocylinders is $m = 0.6$. The number of GST unit structure is seventy-two. The generalized Snell's law is expressed as [42–44]

$$n_i \sin \theta_i - n_t \sin \theta_t = \frac{\lambda}{2\pi} \frac{d\varphi}{dx} \quad (2)$$

where n_i and n_t are the refractive index of incident and refractive sides, respectively. In this work, we suppose both the incident and refractive sides are air. θ_i and θ_t are the incident and refractive angles, respectively, and λ is the incident wavelength in vacuum, $d\varphi/dx$ corresponds to the phase gradient along x direction.

As before, an x -polarized plane wave is supposed normally incident from substrate. We set the period and phase gradient as $2.3 \mu\text{m}$ and $\pi/4$, respectively. After transmitting through the metasurface, a beam will propagate towards the direction with angle of 27.5° . The GST nanocylinders on this metasurface can be designed regarding to the results in Fig. 1(b). To demonstrate, numerical simulation is presented in Fig. 3(a). The electric field distribution shows that the incident light is deflected to the direction with angle of 27.5° , which agrees well with the theoretical values.

In order to obtain more oriented deflection beams with different angles, further optimization on the phase distribution of metasurface is

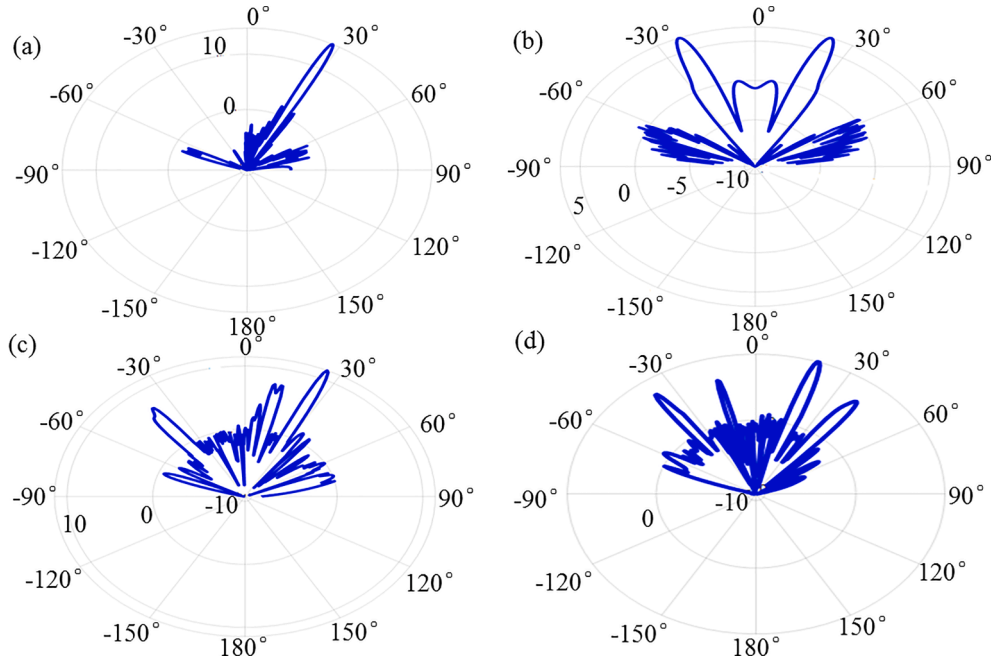


Fig. 4. Far-field radiation pattern calculated from the results in Fig. 3. (a) single beam at angle of 27.5° , (b) two beams at angles of 27.5° and -27.5° , (c) three beams at angles of 17.9° , -38° , and 27.5° , (d) four beams at angles of 17.9° , -17.9° , 38° , and -38° . The unit is dB.

required, which could be achieved by controlling the crystalline fraction of each GST nanocylinder. As examples, we simulated three more cases and plotted the results in Fig. 3(b)–(d). In the first case, the metasurface is divided into two parts and the phase differences between neighboring unit elements are $\pi/4$ and $-\pi/4$, resulting in deflection angles of 27.5° and -27.5° , respectively. Fig. 3(b) depicts the electric field distribution

of the deflected light towards directions with angles of about 27.5° and -27.5° . In the second case, the metasurface is divided into three parts and the phase differences between neighboring unit elements are $\pi/6$, $-\pi/3$ and $\pi/4$, resulting in deflection angles of 17.9° , -38° , and 27.5° , respectively. Fig. 3(c) depicts the electric field distribution of the deflected light towards directions with angles of about 17.9° , -38° , and

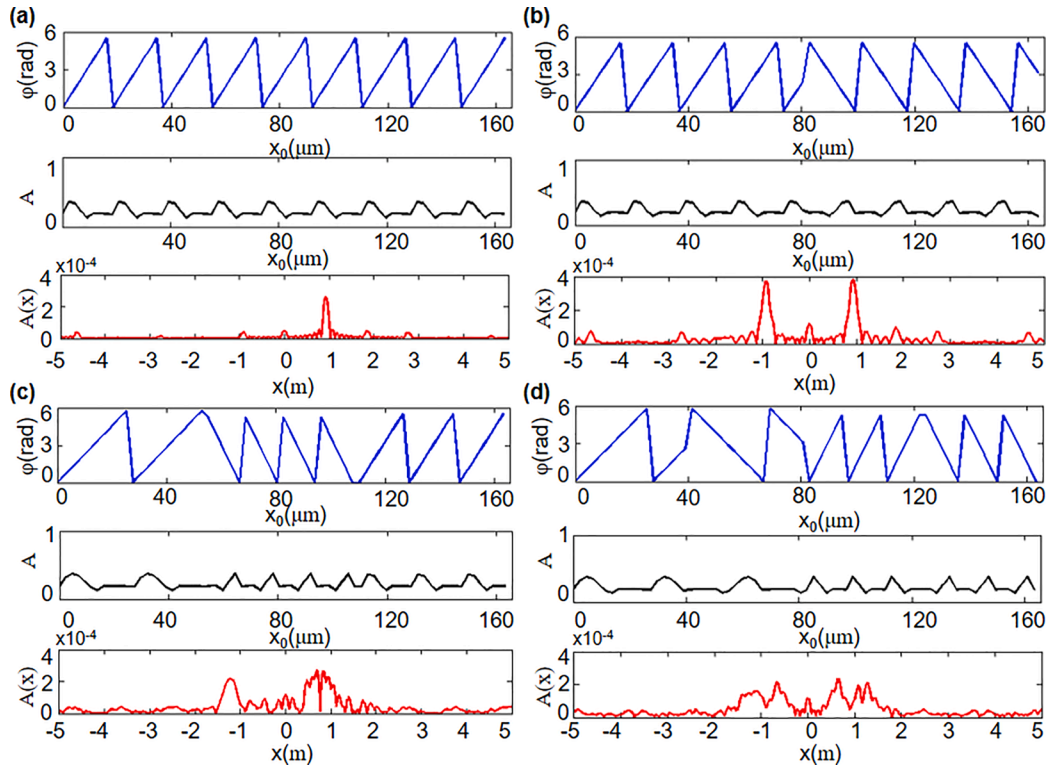


Fig. 5. The deflected light propagating 2 m away is calculated by the Fraunhofer's diffraction formula. (a), (b), (c) and (d) are the results of single deflection angle, two deflection angles, three deflection angles and four deflection angles, respectively. ϕ , A , $A(x)$ represent the phase profile at metasurface, amplitude distribution at metasurface, and amplitude distribution at the distance of 2 m, respectively.

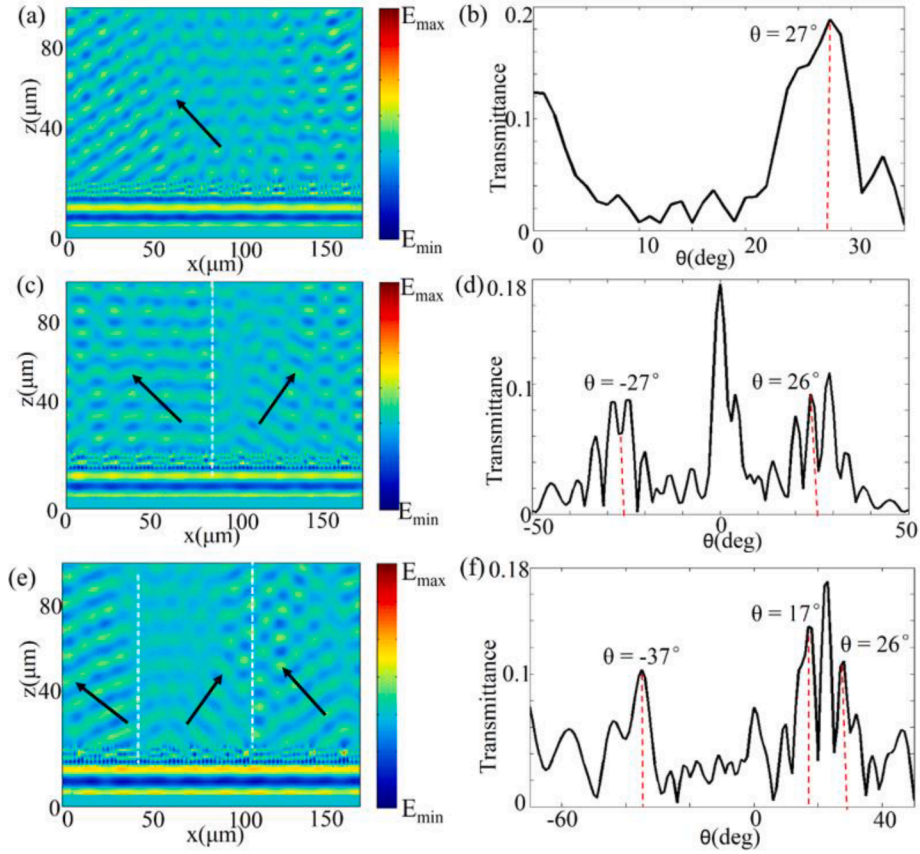


Fig. 6. The deflector is designed at wavelength of $8 \mu\text{m}$, $9 \mu\text{m}$ and $10 \mu\text{m}$. The electric field distribution and transmittance as a function of deflection angle for the case with (a), (b) single beam at wavelength of $8 \mu\text{m}$, with (c), (d) two beams at wavelength of $9 \mu\text{m}$, with (e), (f) three beams at wavelength of $10 \mu\text{m}$. The red dashed lines denote the angles of deflection beams. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

27.5° . In the third case, the metasurface is divided into four parts and the phase differences between neighboring unit elements are $\pi/6$, $-\pi/6$, $\pi/3$ and $-\pi/3$, resulting in deflection angles of 17.9° , -17.9° , 38° , and -38° , respectively. Fig. 3(d) depicts the electric field distribution of the deflected light towards directions with angles of about 17.9° , -17.9° , 38° , and -38° . These simulation results are in good agreements with the theoretical values, and the small deviations between the theory and simulation could be attributed to inaccurate crystalline fraction for each GST cylinder to achieve certain phase profiles.

In addition, we calculated the far-field radiation pattern of the results in Fig. 3. In Fig. 4(a), a single peak with gain of 14.7 dB can be observed at the angle of 27° . Fig. 4(b) shows two peaks with gains of 6.8 dB and 6.75 dB at the angles of 24° and 23.5° , respectively. Fig. 4(c) presents three peaks with gains of 6.9 dB, 7.3 dB and -11.4 dB at angles of 37.6° , 14° and 25.6° , respectively. Fig. 4d shows four peaks with gains of 9.7 dB, 6.3 dB, 6.17 dB and 7.4 dB at the angles of 17.5° , -14.3° , 37.8° and -37° , respectively. The deflection angles in near- and far-field match well, further demonstrating the promising application of our designed metasurface in oriented communication.

To validate, we also studied the performance when the light travels far enough from the oriented deflector. We apply the Fraunhofer's diffraction formula to simulate the amplitude distribution of the deflected beams along x -direction at a propagation distance of 2 m. The Fraunhofer's formula can describes the far-zone properties of a field that has passed through in the metasurface, and can be written as [45]:

$$E(x, y) = \frac{1}{i\lambda z} e^{ik_0(z + \frac{z^2}{2})} \iint E(x_0, y_0) e^{-\frac{ik_0}{z}(x_0 x + y_0 y)} dx_0 dy_0 \quad (3)$$

where E is the electric field, (x, y) and (x_0, y_0) are the coordinates on the

imaging and metasurface planes, respectively, k_0 is the wave vector of the incident light in the vacuum. We use Eq. (3) to calculate the amplitude distributions the above four oriented deflector at a propagation distance of 2 m, and plot the results in Fig. 5. The top, middle and bottom panels of each sub-figure present the phase profile φ at metasurface, amplitude distribution A at metasurface, and amplitude distribution $A(x)$ at the distance of 2 m, respectively. Fig. 5(a) clearly shows that the transmitted light can be orientedly deflected as a single beam after propagating 2 m away. Similarly, we can see from Fig. 5(b) that the deflected light can be divided into two beams towards two opposite directions after propagating 2 m away. Fig. 5(c) and 5(d) are the diffraction results when the transmitted light are deflected into three and four angles, exhibiting three and four separated beams after travelling 2 m distance. These results further confirm that the oriented deflector we designed has great application prospects in oriented communication.

At last, we investigate the broadband performance of our proposed devices. Owing to the tunable optical responses of GST, we may achieve the required phase profiles for different working wavelength by individually engineering the crystalline fraction of each GST nanocylinders. To demonstrate, we keep the metasurface in Fig. 3(a) unchanged and investigate the oriented deflection at wavelengths of $8 \mu\text{m}$, $9 \mu\text{m}$ and $10 \mu\text{m}$. Via tuning optical responses of GST, we try to achieve the deflection of transmitted light into single beams with angle of 27.5° at wavelength of $8 \mu\text{m}$, two beams with angles of 27.5° and -27.5° at wavelength of $9 \mu\text{m}$, and three beams with angles of 17.9° , -38° , and 27.5° at wavelength of $10 \mu\text{m}$. According to the generalized Snell's law, the phase gradient in each case could be calculated. Consequently, we may obtain the required crystalline fraction of GST nanocylinders in each case,

realizing the designed tunable oriented deflector.

Fig. 6 shows the simulation results of the above broadband oriented deflections at wavelength of 8 μm , 9 μm and 10 μm . Fig. 6a shows the electric field distribution at wavelength of 8 μm . Fig. 6b plots the transmittance as a function of deflection angle θ . The simulation results exhibit a single deflection beam with angle of $\theta = 27^\circ$, which is consistent with the theoretical design angle of 27.5° . Fig. 6c and d show the simulation results of two deflection beams with angles of 27.5° and -27.5° at the wavelength of 9 μm . It could be estimated from the simulation results that the deflection angles are $\theta = 26^\circ$ and $\theta = -27^\circ$, well matching the theoretical design angles of 27.5° and -27.5° . The transmission peak at the angle of 0° could be attributed to the interference between the transmitted wave from the right and left parts of the metasurface. Furthermore, we can obtain the deflection angles of $\theta = 17^\circ$, $\theta = -37^\circ$ and $\theta = 26^\circ$ from Fig. 6e and 6f, which are in good agreement with the theoretical angles 17.9° , -38° and 27.5° . The small deviation of simulation from the theoretical design could be attributed to that the crystallization fractions of GST nanocylinders do not perfectly meet the required phase profiles. Overall, it is demonstrated that our approach has significant ability to achieve oriented deflection over a broadband range and has a broad application prospect.

Conclusion

In conclusion, we have successfully demonstrated an oriented focusing metalens and an oriented deflector working at mid-infrared range based on GST metasurface. The dynamically manipulation of the phase profile of the transmission field through the metasurface is realized by artificially controlling the GST crystallization fraction. Both the oriented focusing metalens and the oriented deflector can be achieved without changing the structure but individually engineering the crystalline fraction of each GST nanocylinder. This approach also shows significant ability to achieve oriented deflection over a broadband range. The concept of utilizing the phase change material provides an extra degree of freedom for the phase and wavefront controlling, holding potential applications in oriented communication systems.

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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