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Full 360° terahertz dynamic phase modulation based on doubly resonant graphene-metal hybrid metasurfaces

Bin Xu Wang^{1,2,#}, Xiaoqing Luo^{1,#}, Yalin Lu^{4,5,6*}, and Guangyuan Li^{1,7*}

¹ CAS Key Laboratory of Human-Machine Intelligence-Synergy Systems, Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences, Shenzhen 518055, Guangdong Province, China

² Nano Science and Technology Institute, University of Science and Technology of China, Suzhou 215123, China

³ CAS Key Laboratory of Materials for Energy Conversion, Department of Materials Science and Engineering, University of Science and Technology of China, Hefei 230026, China

⁴ Anhui Laboratory of Advanced Photon Science and Technology, University of Science and Technology of China, Hefei 230026, China

⁵ Synergetic Innovation Center of Quantum Information & Quantum Physics, University of Science and Technology of China, Hefei 230026, China

⁶ Hefei National Laboratory of Physical Science at the Microscale, University of Science and Technology of China, Hefei 230026, China

⁷ Shenzhen College of Advanced Technology, University of Chinese Academy of Sciences, Shenzhen 518055, China

# These authors contribute equally

* Correspondence: gy.li@siat.ac.cn

Abstract: Dynamic phase modulation is vital for tunable focusing, beaming, polarization conversion and holography. However, it remains challenging to achieve full 360° dynamic phase modulation while maintaining high reflectance or transmittance based on metamaterials or metasurfaces in the terahertz regime. Here we propose a doubly resonant graphene-metal hybrid metasurface to address this challenge. Simulation results show that by varying the graphene Fermi energy, the proposed metasurface with two shifting resonances is capable to provide dynamic phase modulation covering a range of 361° while maintaining relatively high reflectance above 20% at 1.05 THz. Based on the phase profile design, dynamically tunable beam steering and focusing are numerically demonstrated. We expect this work will advance the engineering of graphene metasurfaces for the dynamic manipulation of terahertz waves.

Keywords: Graphene; metasurface; phase modulation; terahertz.

1. Introduction

Metasurfaces have attracted increasing attention in the manipulation of the phase, amplitude, polarization, and wavefront of electromagnetic waves due to their appealing merits including compactness, easy integration, and low loss [1–4]. Among these functionalities, the phase modulation is of particular importance [5] since it can lead to diverse relevant applications such as holographic imaging [6], polarization manipulations [7], and wave front control [8,9]. Although various metasurfaces, either based on metals or based on all-dielectrics, have been designed or demonstrated to achieve full 360° phase modulations [1,10], most of these metasurface-based phase modulators are passive devices and cannot be actively tuned after fabrication.

Recently, great efforts have been put on active metasurface-based phase modulation [11–15] by incorporating graphene, stretchable substrates, or phase-change materials such as VO₂ and chalcogenides. Since the first demonstration in 2009 [16], metasurface-based dynamic phase modulators have been of particular interest in the terahertz regime due to the lack of suitable natural

materials. One design strategy is to make use of resonance frequency shifts induced by tuning the material's properties. For example, Zhao *et al.* [17] demonstrated a large phase shift of up to 138° near 0.6 THz using a transmissive VO₂ metasurface, but the transmittance is only 2.5%. Nouman *et al.* [18] demonstrated reconfigurable terahertz phase control based on another VO₂-metal metasurface, and realized a tunable phase shift of 64° and meanwhile relatively high transmittance of 17%. Zhang *et al.* [19] demonstrated large terahertz dynamic phase modulation based on an enhanced resonant active HEMT metasurface, and achieved an experimental 137° dynamic phase shift, but the transmittance is also very low, only less than 5% (or less than -13 dB). On the other hand, based on a graphene-metal hybrid metasurface, Jung *et al.* [20] demonstrated terahertz phase modulators with much higher transmittance of 53%. However, the dynamic phase shift is only 68° . Similarly, Hu *et al.* [21] made use of silicon-metal hybrid metasurface and demonstrated ultrafast terahertz phase modulation with high transmittance of more than 25%. However, the dynamic phase shift is also very limited (only 53°). Therefore, based on transmissive metasurfaces that make use of resonance frequency shifts via tuning the materials, there is a trade-off between the dynamic phase shift and the transmittance, and a large dynamic transmission phase shift above 180° has not been reported yet.

Another widely-adopted design strategy for terahertz phase modulators is to make use of reflective metasurface based on perfect absorption. For example, Miao *et al.* [22] demonstrated a wide phase modulation range of 243° with gate-controlled reflective graphene metasurfaces. Liu and Bai [23] proposed a graphene metasurface and numerically obtained dynamic phase modulation of 180° . Based on graphene metasurfaces Kakenov *et al.* [24] and Tamagnone *et al.* [25] respectively demonstrated voltage controlled terahertz phase modulation of π . Recently, Zhang *et al.* [26] proposed a graphene-metal hybrid metasurface and obtained dynamic phase modulation up to 295° at the frequency of 4.5 THz. Although these reflective metasurfaces based on perfect absorption can achieve much larger dynamic phase range than the transmissive metasurfaces based on resonance frequency shifts, the reflectance is very limited (usually less than 10%).

Therefore, based on the above two design strategies, it remains challenging to achieve full 360° phase modulation while maintaining high transmittance/reflectance. However, in most applications such as tunable metalens [27,28], beam steering [29,30], switchable wave-plates [31,32], and the polarization control [33], dynamic phase modulation covering the full 360° , as well as high reflectance/transmittance is highly desirable. In order to tackle with the challenge of the limited dynamic phase modulation range and relatively low reflectance/transmittance, Zhu *et al.* [34] proposed and demonstrated a multiple resonance metasurface for providing 360° phase variation in the microwave regime. Later, Liu *et al.* [35] proposed a graphene metasurface composed of two resonators to achieve a dynamic 2π phase modulation and meanwhile high reflectance of 56% in the terahertz regime. Similarly, Ma *et al.* [36] also proposed stacked graphene metasurfaces, and numerically obtained dynamic reflection phase covering a range of nearly 2π while maintaining high reflectance in the far-infrared regime. Though these results are encouraging, the two closely packed graphene patch resonators of the terahertz metasurface unit cell in ref. [35] are isolated and thus are difficult to tune the Fermi levels independently.

In this work, we propose a graphene-metal hybrid metasurface based on double resonances in order to achieve full 360° dynamic phase modulation with relatively high reflectance above 20% in the terahertz regime. The metasurface unit cell is composed of gold and graphene hybrid structures built on a reflective substrate sandwiched by a polydimethylsiloxane (PDMS) spacer layer. Distinct from the two closely packed graphene patch resonators in ref. [35], the graphene patches in this work are connected to the source/drain electrode via the gold stripes, facilitating the gate tuning of the Fermi levels of each row of graphene stripes, as illustrate in Figure 1. Simulation results will show that by tuning the graphene Fermi level, the metasurface exhibits two shifting resonances and dynamic 360° phase modulation with relatively high reflectance above 20% at the frequency of 1.05 THz. Based on the phase profile design, a terahertz meta-lens with tunable focusing length and a dynamic beam deflector are numerically demonstrated.

2. Design and Methods

Figure 1 illustrates the proposed graphene-metal hybrid metasurface, which is composed of two gold split-ring resonators (SRRs), two gold stripes, and a graphene patch connecting them. The graphene-gold hybrid structures are built on top of a thick gold film sandwiched with a PDMS spacer layer. The graphene patches are connected to the source/drain electrode via the gold stripes and thus their Fermi levels can be dynamically tuned by gate voltages. The metasurface unit cell has periods of $p_x = p_y = 240 \mu\text{m}$ in both the x and y directions. The two parallel gold stripes have width of $w_s = 4 \mu\text{m}$ and are separated by a distance of $w_y = 228 \mu\text{m}$. The two gold SRRs separated by a gap width of $w_x = 24 \mu\text{m}$ have an outer radius of $R_{\text{out}} = 90 \mu\text{m}$, an inner radius of $R_{\text{in}} = 75 \mu\text{m}$. The vertical bars of the SRRs are separated by a gap of $g = 60 \mu\text{m}$. The graphene stripe connecting the gold stripes and SRRs has widths of $w_x = 24 \mu\text{m}$ and $w_y = 218 \mu\text{m}$ in the x and y directions, respectively. The gold stripes and SRRs have thickness of $t_M = 200 \text{ nm}$, and the PDMS spacer layer has thickness of $t = 45 \mu\text{m}$.

Figure 1. Schematic of the proposed metasurface, the unit cell of which is composed of gold stripes, gold asymmetric split rings and graphene patch on top of a thick gold film sandwiched with a PDMS spacer. (a) 3D view, (b) side view and (c) top view. $p_x = p_y = 240 \mu\text{m}$, $w_s = 4 \mu\text{m}$, $R_{\text{out}} = 90 \mu\text{m}$, $R_{\text{in}} = 75 \mu\text{m}$, $g = 60 \mu\text{m}$, $w_x = 24 \mu\text{m}$, $w_y = 228 \mu\text{m}$, $t_M = 200 \text{ nm}$ and $t = 45 \mu\text{m}$.

The proposed metasurface is illuminated by normally incident terahertz plane wave with electric field polarized along the y axis. The reflectance amplitude and phase spectra, as well as the near-field or far-field distributions were simulated using the frequency domain solver in CST Microwave Studio. Unit cells boundary conditions were adopted in both the x and y directions, and open boundary conditions were used in the z direction. The PDMS spacer was modelled with $\epsilon_r = 2.35$ and $\tan \delta = 0.04$. Gold was modelled using the lossy metal model with the electrical conductivity of $4.561 \times 10^7 \text{ S/m}$. The graphene surface conductivity σ can be decomposed into the interband conductivity σ_{inter} and the intraband conductivity σ_{intra} . In the terahertz regime and at room temperature, the interband contribution can be safely neglected, and thus σ can be approximately expressed as [37,38],

$$\sigma(\omega) = \frac{ie^2 E_F}{\pi \hbar^2 (\omega + i/\tau)}. \quad (1)$$

Here e is electron charge, $\hbar$ is the reduced Plank's constant, E_F is the Fermi energy level of graphene, and τ is the transport relaxation time.

3. Results and Discussion

3.1. Phase modulation performance

Figure 2 depicts the dynamic reflection amplitude and phase spectra of the proposed metasurface with different Fermi levels of graphene. Figure 2a shows that for small graphene Fermi levels of $E_F \leq 0.4 \text{ eV}$, there exists one dominant dip in the reflection spectra; whereas for larger graphene

Fermi levels, an additional dip appears at the higher frequency. The frequencies of both reflection dips increase with the graphene Fermi level: as E_F increases from 0 eV to 1.4 eV, the first dip frequency evolves from 0.93 THz to 1.08 THz, and the second evolves from 1.075 THz to 1.15 THz, as shown by Figure 2ab.

Figure 2. Simulated reflection (a)(b) amplitude and (d)(e) phase spectra for different graphene Fermi levels. Reflection (c) amplitude and (f) phase as functions of graphene Fermi level at 1.05 THz.

The reflection phase spectra are shown in Figure 2d. It is clear that across each reflection dip frequency, the corresponding phase experiences a large shift of 360° . Therefore, at the frequency of 1.05 THz, close to which the two reflection dips appear for different Fermi levels, the reflection phase shift varies continuously, covering a large range of 361° , as graphene Fermi level varies between 0 eV and 1.4 eV, as shown by Figure 2e. On the other hand, the reflection amplitudes are always larger than 0.45. In other words, the dynamic reflection phase modulation reaches up to 361° , and meanwhile the reflectance is above 20%.

To understand the two resonance characteristics of the proposed metasurface, in Figure 3 we plot the surface current maps for $E_F = 0.6$ eV at 1.019 THz and 1.1 THz, and for $E_F = 1.2$ eV at 1.068 THz and 1.136 THz. Given the graphene Fermi level, the two frequencies correspond to the two reflection dips. Results show that for the first resonance at relatively lower frequency, the surface currents are mainly confined to the horizontal gold stripes and the SRRs; whereas for the second resonance at relatively higher frequency, the surface currents are mainly confined to the horizontal gold stripes and the graphene patch. As the graphene Fermi level increases, the surface currents along the graphene patch become stronger.

3.2. Tunable beam deflection

By dynamically controlling the graphene Fermi levels of the metasurface array, we can numerically realize a reflective phased array operating at 1.05 THz for concept proof, as illustrated by Figure 4. The metasurface array is composed of N rows of sub-array along y -axis, and the unit cell of each sub-array can be independently controlled using the gate voltage V_i , $i = 1, 2, \dots, N$. In the simulations, the time domain solver with periodic boundary condition in both x and y directions and open boundary condition in z direction is employed. Under normally incident terahertz plane wave polarized along the

Figure 3. Surface current distributions of the metasurface with two typical graphene Fermi levels of (a)(b) 0.6 eV for (a) 1.019 THz and (b) 1.1 THz, and (c)(d) 1.2 eV for (c) 1.068 THz and (d) 1.136 THz.

y -axis, the anomalous reflection wavefront is deflected from the metasurface normal with a deflection angle of θ following the generalized Snell's law equation [39],

$$\theta = \sin^{-1} \left(\frac{\lambda}{2\pi} \frac{\Delta\phi}{\Delta y} \right), \quad (2)$$

where λ is the operation wavelength, and $\Delta\phi$ and Δy are the phase difference and the geometric distance between the neighboring unit cells, respectively.

Figure 4. (a) Schematic of the phased array structure for achieving dynamic reflection beam steering. (b) Reflection phase distributions of the designed phased array for achieving four specific deflection angles.

As an example, we designed four deflection angles, $\theta = -5^\circ$, -11° , -17° and -23° . The distance between two neighbouring unit cell is $\Delta y = 240 \mu\text{m}$. According to Equation (2), the corresponding phase differences between the neighbouring unit cells should be $\Delta\phi = \pi/6$, $\pi/3$, $\pi/2$, and $2\pi/3$, respectively. Thus, theoretical numbers of unit cells in each sub-array are $N = 12$, 6, 4, and 3,

respectively. Figure 4b shows the required phase profile with $\phi_i = i\Delta\phi$ with $i = 1, 2, \dots, N$ for the four designed deflection angle. As it is not practical to have smooth phase variations, we adopted discrete phase points to approximate the continuous phase profile. In simulations, the graphene Fermi levels corresponding to these reflection phase points can be determined by their quasi-linear relationship as shown in Figure 2f.

Figure 5. (a)–(d) Near-field electric field distributions $|E_x|$ and (e)–(h) far-field directivity for deflected reflection angle of (a)(e) $\theta = -5^\circ$, (b)(f) -11° , (c)(g) -17° and (d)(h) -23° .

Figure 5 depicts the simulated near-field electric field distributions and the far-field directivity for the designed four deflection angles. Results show that anomalous reflection angles of -5° , -11° , -17° and -23° are clearly observed through the E-field pattern in Figure 5a–d, respectively. There are some distortions on the wavefront, which correspond to sidelobes in the far-field directivity, as shown by Figure 5e–f. We find that the directivity differences between the main lobe and the side lobes for the designed four deflection angles reach 7.5 dB, 8.2 dB, 9.6 dB and 6.8 dB, respectively.

Note that according to Equation (2), the signs of the deflection angles can also be flipped by reversing the phase point of each unit cell. Moreover, when $\Delta\phi = 0$, which can be done by setting the same gate voltage or the same graphene Fermi level for all the unit cells, the reflection wavefront is not deflected, i.e., $\theta = 0$. For the sake of simplicity, these results are not shown here.

3.3. Tunable focusing

Given the same arrayed metasurfaces as illustrated by Figure 4a, we can also realize tunable reflection focusing at 1.05 THz. As a proof of concept, we illustrate the tuning focusing with three different focal lengths of $F = 5$ mm, 5.5 mm, and 6 mm. For this purpose, the phase distribution of the array should be [1]

$$\phi(y) = \frac{2\pi}{\lambda} \left(\sqrt{F^2 + y^2} - F \right), \quad (3)$$

where F is the designed focal length. The desired phase profiles calculated with Equation (3) for the three designed focal lengths at 1.05 THz are depicted by the blue curves in Figure 6d–f, respectively. In simulations, each of these phase profiles are replaced by 37 discrete phase points that are given by

$$\phi(m) = \frac{2\pi}{\lambda} \left(\sqrt{F^2 + (md)^2} - F \right), \quad (4)$$

Figure 6. (a)–(c) Electric field intensity distributions $|E_x|^2$, and (d)–(f) desired phase profiles (blue curves) and discrete phase points of the focusing metasurface array with designed focal lengths of (a)(d) $F = 5$ mm, (b)(e) 5.5 mm and (c)(f) 6 mm operating at 1.05 THz.

where $y = md$ with $m = 0, \pm 1, \pm 2, \dots, \pm 18$ is incorporated for discretization. In the simulations, the time domain solver with periodic boundary condition in the x direction and open boundary condition in the y and z directions is adopted.

The red circles in Figure 6d–f show these discrete phase points. Figure 6a–c shows strong focusing effect of the reflected beams with the designed focal lengths of 5 mm, 5.5 mm and 6 mm can be observed, consistent with our expectation. The focused electric fields are greatly enhanced.

Figure 7. Normalized electric field intensity along y -axis (when z locates at the focal points) for (a) $F = 5$ mm, (b) 5.5 mm and (c) 6 mm, respectively.

To quantify the focusing quality, the electric field intensity along the y -axis when z is fixed to the focal point is extracted and is shown in Figure 6. The calculated spot sizes, *i.e.*, the full width half maximums (FWHMs), are all approximately equal to $215 \mu\text{m}$. This corresponds to $0.75\lambda_0$ for

$\lambda_0 = 285.7 \mu\text{m}$ (1.05 THz). Therefore, we find that the focusing intensities, as well as the spot sizes are almost constant for these three different focal lengths. These characteristics are appealing in practical applications.

4. Conclusion

In conclusion, we have numerically demonstrated full 360° dynamic phase modulation while maintaining relatively high reflectance above 20% in the terahertz regime based on a reflective graphene-metal hybrid metasurface with double resonances. The Fermi level of the graphene patch within the metasurface unit cell can be actively tuned by controlling the gate voltage. Results have shown that, at the frequency of 1.05 THz, around which two resonances can appear for different graphene Fermi levels, this remarkable dynamic phase modulation performance can be achieved. Based on the phase profile design, we have further numerically demonstrated tunable steering within the angle range of $\pm 23^\circ$, and a terahertz metalens with tunable focal lengths within $5 \sim 6 \text{ mm}$. Therefore, the presented graphene-metal hybrid metasurfaces could provide solutions to the active manipulation of terahertz waves in applications such as terahertz imaging, holography, and telecommunications.

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