Multifunctional Metasurfaces
Design Principles and Device Realizations
Synthesis Lectures on Materials and Optics

Multifunctional Metasurfaces: Design Principles and Device Realizations
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Multifunctional Metasurfaces
Design Principles and Device Realizations

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ABSTRACT
In recent years, we have witnessed a rapid expansion of using super-thin metasurfaces to manipulate light or electromagnetic wave in a subwavelength scale. However, most designs are confined to a passive scheme and monofunctional operation, which hinders considerably the promising applications of the metasurfaces. Specifically, the tunable and multifunctional metasurfaces enable to facilitate switchable functionalities and multiple functionalities which are extremely essential and useful for integrated optics and microwaves, well alleviating aforementioned issues. In this book, we introduce our efforts in exploring the physics principles, design approaches, and numerical and experimental demonstrations on the fascinating functionalities realized. We start by introducing in Chapter 2 the “merging” scheme in constructing multi-functional metadevices, paying particular attention to its shortcomings issues. Having understood the merits and disadvantages of the “merging” scheme, we then introduce in Chapter 3 another approach to realize bifunctional metadevices under linearly polarized excitations, working in both reflection and transmission geometries or even in the full space. As a step further, we summarizes our efforts in Chapter 4 on making multifunctional devices under circularly polarized excitations, again including designing principles and devices fabrications/characterizations. Starting from Chapter 5, we turn to introduce our efforts on using the “active” scheme to construct multifunctional metadevices under linearly polarized wave operation. Chapter 6 further concentrates on how to employ the tunable strategy to achieve helicity/frequency controls of the circularly polarized waves in reflection geometry. We finally conclude this book in Chapter 7 by presenting our perspectives on future directions of metasurfaces and metadevices.

KEYWORDS
multifunctional metasurface, polarization-dependent, helicity control, tunable, full-space, geometric phase, propagation phase, reflection, transmission
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CHAPTER 1

Introduction

Manipulating electromagnetic (EM) waves in the desired manners is one of the most important tasks in photonics research, as photons are believed to be alternative information carriers that may play crucial roles in the next-generation industry revolution. According to Maxwell's equations, permittivity and permeability of a medium dictate the behaviors of EM waves propagating inside it. However, naturally existing materials only exhibit limited abilities to control EM waves, since their permittivity $\varepsilon$ lie in a narrow variation range and even worse, their permeability $\mu$ are all very close to 1 at high frequencies (e.g., the visible range), due ultimately to the weak interactions between natural molecules/atoms and magnetic fields of EM waves. As a result, typically conventional EM devices need to be thick enough (compared to the operation wavelength) and exhibit certain curved shapes to ensure appropriate propagation phases accumulated, to realize the desired wave-manipulation functionalities (say, focusing). Besides, efficiency is also an issue for conventional devices caused by an impedance mismatch between air and natural materials which typically do not exhibit magnetic responses. Such limitations (i.e., size, shape, and efficiency) significantly hinder the applications of conventional optical devices in next-generation on-chip photonics scenarios which are typically flat, ultra-compact, and energy saving. Meanwhile, facing the increasing demands on data-storage capacity and information processing speed in modern science and technology, EM integration plays a more and more important role and has attracted intensive attention with remarkable applications. An ultimate goal pursued by scientists and engineers along this development is to make miniaturized devices as small as possible yet equipped with powerful functionalities as many as possible. However, available efforts based on conventional materials suffer from the issues of device thickness, low efficiency, and restricted functionalities.

Metamaterials (MTMs) \cite{1, 2}, consisting of deep-subwavelength-sized EM microstructures (e.g., meta-atoms) arranged in periodic or non-periodic orders, have drawn much attention recently. Through tailoring the microstructures of meta-atoms, MTMs can in principle exhibit arbitrary values of $\varepsilon$ and $\mu$, thus exhibiting extraordinarily strong capabilities to control EM waves. Many fascinating wave-manipulation effects have been demonstrated based on MTMs, such as negative refraction \cite{3, 4}, super-resolution imaging \cite{5, 6}, cloaking \cite{7–9}, polarization-control \cite{10–13}, perfect light absorption \cite{14}, and transparency \cite{15, 16}, and unusual wave-control effects realized by zero-index MTMs \cite{17, 18}. Attempts have also been made to achieve multifunctional EM devices based on MTMs. However, the realized devices typically exhibit bulky sizes and low efficiencies, since MTMs are three-dimensional (3D) materials composed...
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by resonant metallic structures which can easily absorb EM waves. Moreover, such 3D devices require complex fabrication processes, adding more disadvantages to EM integrations [19, 20].

Metasurfaces, ultrathin MTM layers constructed by planar meta-atoms of predetermined EM responses arranged in specific two-dimensional (2D) orders, can largely overcome the difficulties faced by MTMs. In recent years, we have witnessed a rapid development of using ultrathin metasurfaces to manipulate light or EM waves on deep-subwavelength scales. Tuning the EM responses of meta-atoms to realize certain transmission/reflection phase distributions on the metasurfaces, one can use these ultra-thin devices to efficiently reshape the wavefronts of incident EM beams based on Huygens’ principle, achieving unusual effects including anomalous beam bending based on generalized Snell’s law [21–29], propagating wave to surface waves conversion [30–32], polarization-control [33–39], focusing [40–42], holograms [43–45], flat-lens imaging [46–50], tunable devices [51–53], photonic spin–Hall effect [54–56], etc. In contrast to MTM-based EM devices replying critically on the propagation phases of EM waves, metasurfaces fully exploited the abrupt phase changes of EM waves at the meta-atom interfaces, and therefore, they can be much thinner than the working wavelength. Meanwhile, since typically EM waves do not stay inside metallic structures for a long time, the loss issue can be significantly alleviated in metasurface-based devices. Also, the flat configuration makes such systems easy to fabricate. Most importantly, by tailoring the “order” on which the meta-atoms are arranged, one can realize metasurfaces exhibiting desired inhomogeneous distributions of amplitude and phase for transmitted/reflected EM waves, enabling diversified fascinating wave-manipulation effects far beyond those realized with MTM-based devices.

These unique features make metasurfaces ideal candidates to realize flat and miniaturized metadevices exhibiting powerful wave-manipulation capabilities, being particularly suitable for on-chip photonic applications. Typically, the devices made by metasurfaces are flat, much thinner than the wavelength, and exhibit much higher efficiencies than their bulky MTM counterparts, all being highly favorable for integration-optics applications. These attractive properties make metasurfaces the best candidates to construct multifunctional EM devices. Indeed, many efforts have recently been devoted to designing multifunctional optical devices based on metasurfaces, typically using polarization, helicity, frequency, or incidence angle of the impinging light as external knobs to control the functionalities exhibited by the devices. The proposed/demonstrated devices are usually equipped with functionalities combining two or more of those demonstrated before on single-function metasurfaces, such as beam bending, focusing, hologram, surface-wave conversion, directive beaming, etc. In what follows, we briefly summarize the available mechanisms so far developed to realize multifunctional metadevices.

1. Polarization is one important degree of freedom that can be used to realize multifunctional metadevices. Based on anisotropic meta-atoms with polarization-sensitive EM responses, various metadevices were realized at different frequencies, exhibiting multiple functionalities triggered by incident EM waves with different linear polarizations (LPs) [57–63]. In 2014, a dual-functional meta-hologram was experimentally demonstrated based on
anisotropic metal–insulator–metal (MIM) meta-atom [64]. However, the device still exhibits similar functionalities (e.g., hologram) for two incident polarizations. In 2016, a general strategy was proposed to design bifunctional metadevices exhibiting distinct functionalities with very high efficiencies [57]. Very recently, such a concept was successfully implemented in the optical regime [59]. For transmissive metadevices, in addition to using multilayer meta-atoms, Huygens’ meta-atoms and dielectric meta-atoms were also frequently adopted to construct multifunctional metadevices with distinct functionalities in the near-infra-red (IR) regime [65].

2. Helicity is another degree of freedom frequently exploited to design multifunctional metadevices based on the Pancharatnam–Berry (PB) mechanism [66–73]. A commonly applied scheme is to merge several different PB metasurfaces, each exhibiting a certain functionality as the incident circular-polarized (CP) light takes a particular helicity, into one single device [70, 71]. Although such a “merging” strategy is physically straightforward, realized devices exhibit limited working efficiencies and suffer from the issue of functionality cross-talking. In 2015, PB metasurfaces were proposed to record various hologram patterns into helicity-multiplexing channels [66]. While the realized hologram exhibits broadband properties, the measured working efficiency was very low. Recently, Hasman’s group experimentally demonstrated that the alliance of spin-enabled geometric phase and shared-aperture concepts can open a new pathway to implement photonic spin-controlled multifunctional metasurfaces [73, 74]. Helicity-controlled multiple wavefronts such as vortex beams were demonstrated in the visible regime [67]. Combining geometric and propagating phases, chiral holograms were experimentally demonstrated based on transmissive dielectric metasurfaces, which can efficiently generate independent far-field images for right circular polarization (RCP) and left circular polarization (LCP) excitations [68].

3. Wavelength-multiplexing is also widely exploited to realize multifunctional metasurfaces. In 2016, multicolor meta-holography was experimentally realized with a single type of plasmonic pixel, based on an off-axis illumination method [75]. In a parallel line, dielectric metasurfaces were used to build high-efficiency wavelength-multiplexing metadevices at optical frequencies, based upon carefully designed silicon nano blocks [76]. Again, the experimentally achieved efficiencies of the reconstructed images for highly dispersive color holograms are limited due to the intrinsic issue of the “merging” concept.

4. Incidence angle was recently identified as another degree of freedom to be exploited. In 2017, Kamali et al. proposed an angle-multiplexed metasurface, composed of reflective high dielectric contrast U-shaped meta-atoms with incidence-angle-sensitive responses, and experimentally demonstrated that it can realize high-efficiency angle-multiplexed diffractions and holograms at the working wavelength of 915 nm [77]. Zhou’s group established a theory to quantitatively describe the angular dispersion in metasurfaces [78] and
propose a general strategy to realize angle multiplexed metadevices [79], which can exhibit distinct wave-front-control functionalities as shined at different incident angles. Such angle multiplexed metadevices are realized through carefully controlling both the near-field couplings between meta-atoms and the radiation pattern of a single meta-atom.

Adding “active” elements into metasurfaces is another important approach to achieve multifunctional metadevices, with functionalities controlled by external stimuli. Such an “active” scheme stimulates a lot of research works recently, forming a very “active” research sub-field. Below we briefly mention several representative approaches, categorized based on the external stimuli used.

5.1 **Electrically sensitive materials** include varactor diodes, liquid crystals, doped semiconductors, and 2D materials, functioning in different frequency regimes. At microwave frequencies, varactor and PIN diodes are frequently adopted in designing tunable metasurfaces [80–84], since their EM responses (e.g., capacitances) can be dramatically tuned by applying external voltages. In THz and IR regimes, doped semiconductors are often used, since their conductivities (and thus optical responses) can be dramatically modified via electrical gating. Such a mechanism features broad bandwidth and high modulation speed and is compatible with C-MOS technology [85–91]. Graphene, a zero-bandgap 2D material with conductivity tuned efficiently via external gating, is another excellent candidate to help realize tunable devices in the THz or mid-IR regimes, typically in combination with carefully designed metasurfaces [92–107]. Liquid crystals are also widely used as “active elements,” since the orientation angles of molecules such media can be controlled by external electric fields, leading to significant modulations on the refractive index. Resonant properties of metasurfaces with liquid crystals incorporated can thus be efficiently tuned by applying the electric field across the liquid crystals [108–110].

5.2 **Optically sensitive materials (OTMs)** can be hybridized with passive metasurfaces to realize tunable multifunctional metadevices. OTMs include semiconducting materials and optically responsible phase-change materials, whose optical properties strongly depend on the pumping light. Combining these OTMs with carefully designed meta-atoms, various functionality-tunable metadevices were realized by different groups in different frequency regimes [111–117].

5.3 Exerting **mechanical forces** on a metasurface can also efficiently tune its optical properties since the meta-atom structure or its local environment can be dramatically modified. Micro-electro-mechanical-system (MEMS) or nano-electro-mechanical-system (NEMS) are widely used technologies to realize mechanically tunable metasurfaces in different frequency domains [118–124]. Mechanically tunable metasurfaces based on stretchable and flexible substrates have been proposed to achieve var-
ious dynamic effects (e.g., color tuning [125, 126], switchable holograms [127], and varifocal lenses [128]).

5.4 Incorporating thermally responsive materials into metasurfaces is another approach to realizing tunable metasurfaces. Vanadium dioxide (VO2) [129, 130], liquid crystals, and superconductors [131, 132]) are typical examples of this class, which exhibit temperature-dependent optical properties. Therefore, these materials were also frequently adopted to design tunable metadevices exhibiting different functionalities [129–135].

5.5 In addition to the mechanisms introduced above, many others have also been successfully used to realize tunable metadevices in different frequency ranges. For example, one can incorporate ferroelectric materials into the meta-atom design, which can be tuned by applying a magnetic field [136]. Liu et al. demonstrated a kind of dynamic plasmonic color display technology that can realize tunable metadevices based on a chemical approach [137]. Controlled hydrogenation and dehydrogenation of the constituent magnesium nanoparticles, which serve as dynamic pixels, allow for plasmonic color printing, tuning, erasing, and restoration of color.

Having briefly mentioned existing approaches in making multifunctional metadevices, in this book, we would like to summarize our efforts devoted to this fast-developing field in the past several years. To benefit our readers, we will introduce the physics principles and design approaches of these metadevices, in addition to presenting the numerical and experimental demonstrations on the fascinating functionalities realized. This book is organized in the following way. We start by introducing in Chapter 2 the “merging” scheme developed in the early years and widely adopted by several groups in constructing multi-functional metadevices, paying particular attention to its shortcomings issues (e.g., low operating efficiencies and functionality cross-talking). Having understood the merits and disadvantages of the “merging” scheme, we then introduce in Chapter 3 another approach to realize bifunctional metadevices under LP excitations, working in both reflection and transmission geometries or even in the full space. In addition to presenting several high-efficiency metadevices experimentally demonstrated with various combinations of functionalities, we focus on the working principle and design approach to achieve such devices, including how to diminish the cross-talkings between different functionalities. Chapter 4 summarizes our efforts on making multifunctional devices under CP excitations, again including designing principles and devices fabrications/characterizations. Starting from Chapter 5, we turn to introduce our efforts on using the “active” scheme to construct multifunctional metadevices. Specifically, we first introduce in Chapter 5 the design principles to realize such tunable metadevices under LP excitations and then present several proof-of-concept demonstrations of metadevices in both reflection and transmission geometries exhibiting switchable wave-control functionalities. Next, concentrate on how to employ the tunable strategy to achieve helicity/frequency controls of the CP waves in reflection geometry (Chapter 6). We
finally conclude the book in Chapter 7 by presenting our perspectives on future directions of metasurfaces and metadevices.
CHAPTER 2

Early Attempts on Multifunctional Metasurfaces: The “Merging” Concept

2.1 DESIGN PRINCIPLES

Facing increasing demands on speed and memory of EM devices, EM integration is highly desired in modern science and technology. Metasurfaces are ideal candidates to integrate multiple diversified functionalities into single devices with deep-subwavelength thickness and high efficiencies [138]. Various approaches have recently been proposed to achieve this goal, and a simple and physically straightforward scheme developed in the early years utilized the so-called “merged” meta-structures to achieve multifunctional metasurfaces. In such a scheme, people first design individual metasurfaces exhibiting their functions (e.g., one for holographic image and one for vortex beam) and then construct a multifunctional device simply through merging the two structures. Below we present several examples to illustrate how the scheme works.

In order to introduce the “merging” concept more clearly, we take a typical bifunctional metasurface based on the “merging” concept as an example. Figure 2.1 presents an optical bifunctional metasurface that can realize a hologram image or a vortex beam, depending on the helicity of excitation light [139]. To achieve their end, the authors first design two individual metasurfaces (both utilizing the metal-bar structure as basic meta-atoms) which can realize one of the needed functionalities when they are shined by incident light taking circular polarization (CP) with different helicities (see Fig. 2.1). The desired phase profiles on two metasurfaces are created by the PB principle [54, 140] through rotating the metallic bars at different positions by appropriate angles. Since the two metasurfaces exhibit identical periodic structures and there are enough open spaces between metallic bars, the authors then merge two metasurfaces to obtain the final design in which all metallic bars do not touch with each other. Such a device was finally fabricated out and experimentally characterized, showing nice bifunctional performances (Fig. 2.1). However, the working efficiency of the device is quite low, which is found to be around 9% [139].
2. EARLY ATTEMPTS ON MULTIFUNCTIONAL METASURFACES

Figure 2.1: Multifunctional device designed with merged structures. Design strategy, sample picture, and experimental characterizations of a multifunctional metasurface than can generate holographic images or a vortex beam depending on the helicity of incident circularly polarized light.

2.2 REFLECTION-GEOMETRY REALIZATIONS

Having understood the key issues in the “merging” concept, based on which people designed kinds of multifunctional metasurfaces and first is in reflection geometry because high-efficiency reflective meta-atoms are much easier to find than their transmissive counterparts.

Wen et al. further experimentally demonstrated a design methodology to achieve helicity multiplexed functionalities by combining two sets of hologram patterns operating with opposite incident helicities on the same metasurface \[141\]. First, the Gerchberg–Saxton algorithm is used to generate two-phase profiles, which can reconstruct two off-axis images on the different sides of the incident light. Both images (“bee” and “flower”) have a projection angle of $22^\circ \times 22^\circ$ and an off-axis angle of $10.35^\circ$ in the imaging area. Then, the two-phase profiles are encoded onto the metasurfaces (Fig. 2.2a), where the $n$th phase pixel $\psi_n$ of the hologram is represented by a nanorod with the orientation angle $\psi_n/2$ defined in the metasurface. After that, two sets of data are merged with a displacement vector of $(d/2, d/2)$, as shown in Fig. 2.2a. $d$ is the distance between neighboring antennas with a value of 424 nm. Therefore, although the new metasurface contains two sets of hologram data, the size of the sample is still the same and the equivalent pixel size is $300 \times 300$ nm, leading to an increase of the nanoantenna density. On the illumination of left circular polarization (LCP) light, the merged metasurface can reconstruct the ‘flower’ on the left and the “bee” on the right side of the metasurface viewing from the incident
2.2. REFLECTION-GEOMETRY REALIZATIONS

Figure 2.2: (a) A metasurface that can generate multiple hologram images as shined by circularly polarized light with different helicity. (b) Schematic and scanning electron microscope image of the metahologram for projecting the polarization-controlled dual images of “NTU” and “RCAS.”

beam, respectively (Fig. 2.2a). Since the sign of the phase profile can be flipped by controlling the helicity of the incident light, the positions of reconstructed images in Fig. 2.2a are swapped in contrast to those in Fig. 2.2a when the helicity of the incident light is changed from LCP to right circular polarization (RCP).

As a result, the reconstructed images on the same position are switchable, that is, either “bee” or “flower,” depending on the helicity of the incident light.

Tsai's group presented a reflection-type metahologram for visible light that can overcome the issues mentioned above [64]. The basic meta-atoms are MIM structures with the top resonators being gold nanocrosses, which inherently possess much higher efficiencies than the V-antennas proposed by Shalaev's group [142]. By tuning the structural details, one can easily obtain a set of meta-atoms that yield different reflection phases to cover the full $2\pi$ range, yet with reflection, amplitudes staying at high values. Moreover, the lengths of two orthogonal nanorods are free parameters to independently control the reflection phases for two LPs, which
2. EARLY ATTEMPTS ON MULTIFUNCTIONAL METASURFACES

allowed the authors to design a single metasurface encoding two distinct hologram images (i.e., “NTU” and “RCAS”) when illuminated by light with different polarizations (see Fig. 2.2b). The realized metaholograms can work within broadband (width ≈ 880 nm) under a wide range of incident angles. The measured efficiency of the device is about 18% at the wavelength of 780 nm, while the simulated value is even higher (28%). Compared to the transmission-type metaholograms [142], this scheme yields much higher efficiency and does not require polarization conversion for detection. The working efficiency can be further improved by introducing more phase levels and reducing material losses.

2.3 TRANSMISSION-GEOMETRY REALIZATIONS

Such a “merging” concept has been straightforwardly applied to realize many other transmission-geometry multifunctional metadevices.

Similar to the reflection-geometry realizations mentioned above, a commonly applied scheme is to merge several different PB metasurfaces, each exhibiting a certain functionality as the incident CP light takes a particular helicity, into one single device [71], which is shown in Fig. 2.3a. In 2015, Huang et al. proposed to use PB metasurfaces to record various hologram patterns into helicity-multiplexing channels, as shown in Fig. 2.3c [66]. Although a broadband hologram ranging from 633–1000 nm was experimentally achieved, the measured working efficiency was only 4.5% at 810 nm (0.65% at 1000 nm).

The transmission-geometry multifunctional metadevices can work tools for polarization imaging and image processing [143, 144]. Chen’s group experimentally demonstrated a light sword metasurface lens with multiple functionalities. As shown in Fig. 2.3b, the position of focal segments can be controlled by changing the polarization state of the incident light [143]. To design such a multifunctional device, two metasurfaces (each one for a specific focal segment) are designed to operate with opposite incident helicities and merged with a displacement. The conversion efficiency between the polarization states based on the plasmonic metasurface is measured to be 2% at 650 nm, which is at the lower edge of what is required for practical applications.

Yang’s group experimentally demonstrate chiral geometric metasurfaces based on intrinsically chiral plasmonic stepped nanoapertures with a simultaneously high circular dichroism in transmission and large cross-polarization ratio in transmitted light to exhibit spin-controlled wavefront shaping capabilities [145]. As shown in Fig. 2.3d, the chiral geometric metasurfaces are constructed by merging two independently designed subarrays of the two enantiomers for the stepped nanoaperture. Under a certain incident handedness, the transmission from one subarray is allowed, while the transmission from the other subarray is strongly prohibited. The merged metasurface then only exhibits the transmitted signal with the phase profile of one subarray, which can be switched by changing the incident handedness. Based on the chiral geometric metasurface, both chiral metasurface holograms and the spin-dependent generation of hybrid-
Figure 2.3: (a) Schematic to show the polarization selectivity of the metasurface device. The metasurface functions as a hologram to reconstruct an image of “cat” or a lens that converges the incident light into the focal point, depending on the incident/detected light combination. (b) Schematic of multifunctional light sword metasurface lens. Upon the illumination of incident light with linear polarization (LP), the device has two real focal segments corresponding to the transmitted light with RCP and LCP. (c) Schematic illustration of the hybrid multiplexing holograph based on PB Metasurfaces. (d) Illustration of the chiral metasurface hologram merging subarray A and subarray B to enable spin-controlled wavefront shaping. Subarrays A and B are contributing to the images of “owl” and “window,” respectively. Reconstructed images for the chiral metasurface hologram at 820 nm for different polarization states. (e) 3D views of all-silicon supercells and scanning electron microscope image of the fabricated metasurface. The schematic illustration of the designed devices that generate diffraction patterns in the transmission (or reflection) field under the illumination of LCP (or RCP). (f) Dielectric wavelength-multiplexed metasurfaces for achromatic and dispersive holograms.
2. EARLY ATTEMPTS ON MULTIFUNCTIONAL METASURFACES

Order Poincaré sphere beams are experimentally realized. When the chiral geometric metasurface is switched on, the holography efficiency is measured to be 6.8% at 820 nm.

As an alternative to metallic nanorods, however, a dielectric metasurface can be used to dramatically increase this value since it can decrease the ohmic losses and improve the scattering cross-sections of the metal nano-rods. An all-dielectric monolayer metasurface is proposed by Luo’s group to simultaneously realize circular asymmetric transmission (AT) and wavefront shaping based on asymmetric spin-orbit interactions (Fig. 2.3e) [146]. Circularly polarized incidence, accompanied by arbitrary wavefront modulation, experiences spin-selected destructive or constructive interference. An extinction ratio of ≈ 10 : 1 and an AT parameter of ≈ 0.69 at 9.6 μm, as well as a full-width half-maximum of ≈ 2.9 μm (∼ 30% of the peak wavelength), is measured with the designed metasurface. As far as it is known, this is the first report on the realization of simultaneous giant AT and arbitrary wavefront modulation with only one metasurface. In a parallel line, other dielectric metasurfaces are used to build high-efficiency wavelength-multiplexing metadevices at optical frequencies. As shown in Fig. 2.3f, Wang et al. experimentally demonstrated that a metasurface formed by three kinds of silicon nano blocks multiplexed in a subwavelength super-unit can achieve wavefront manipulations for red, green, and blue light, simultaneously [76].

2.4 ISSUES WITH THE “MERGING” SCHEME

In reviewing these metadevices based on the “merging” concept, we find that the proposed design strategy is physically transparent and easy to implement. However, to make the “merging” process work, the adopted meta-atoms must be very simple structures (say, metal bar) to avoid metallic overlapping. Unfortunately, these meta-atoms typically do not satisfy the 100%-efficiency criterion established for PB metasurfaces [54], and thus one type of meta-atoms can generate background noises in addition to the desired functionalities. As a result, such metadevices typically suffer from the issues of low operating efficiencies and functionality cross-talking, except [141] where the issue was partially solved by seeking a high-efficiency PB meta-atom in reflection geometry. Although the dielectric metasurface can decrease the ohmic losses and improve the scattering cross-sections [76, 146], the experimentally achieved working efficiencies of the are also limited due to the intrinsic issue of the “merging” concept. In conclusion, such a “merging” strategy is physically straightforward but the realized devices exhibit limited working efficiencies and suffer from the issue of functionality cross-talking.
While the “merging” scheme described in the last section is simple and easy to implement, it faces several severe issues that limit its practical applications, as discussed at the end of the last section. In this chapter, we propose an alternative strategy to design high-efficiency bifunctional metasurfaces in responses to EM waves with LPs [57, 58, 61], based on single-structure meta-atoms with anisotropic EM properties. We first present the working principles of such high-efficiency bi-functional metasurfaces working in reflection, transmission, and even full-space geometries, respectively. Based on the derived criteria for different cases, we next introduce the designs and fabrications of several bifunctional metadevices and employ microwave experiments, including far-field and near-field properties, to demonstrate their pre-designed bi-functionalities.

3.1 DESIGN PRINCIPLES: EFFICIENCY AND POLARIZATION CROSS-TALK

We first present our design principle to realize multi-functional metadevices/metasurfaces with high efficiencies [57, 58]. In this chapter, the multifunctional metasurfaces are excited in linear-polarizations, and the system exhibits global mirror symmetries with respect to $x \rightarrow -x$ and $y \rightarrow -y$ operations. The EM characteristics of those meta-atoms can be described by two diagonal Jones’ matrices:

$$ R(x, y) = \begin{pmatrix} r_{xx}(x, y) & 0 \\ 0 & r_{yy}(x, y) \end{pmatrix} $$
3. MULTIFUNCTIONAL METASURFACES/METADEVICES

and

\[ T(x, y) = \begin{pmatrix} t_{xx}(x, y) & 0 \\ 0 & t_{yy}(x, y) \end{pmatrix}. \]

with \( r_{xx}, r_{yy}, t_{xx}, t_{yy} \) being the reflection/transmission coefficients for waves polarized along two principal axes \( \hat{x} \) and \( \hat{y} \) for each meta-atom. To achieve high efficiency for the metasurface working in reflection geometry, we need a reflective metasurface with \( T \equiv 0 \) and \(|r_{ii}(x, y)| = 1\). For transmission geometry, a totally transmissive meta-atoms with \( R \equiv 0 \) and \(|t_{ii}(x, y)| = 1\) should satisfy. While in order to realize high-efficiency metasurfaces working in full-space conditions, we need our meta-atoms to be perfectly reflective and transparent for two orthotropic polarizations, such as totally reflective for an \( \hat{x} \)-polarized incidence and perfectly transparent for a \( \hat{y} \)-polarized case. Moreover, in all cases, the corresponding phases with non-zero coefficients should be freely tuned within a \( 2\pi \) variation range by varying the structural parameters of the meta-atoms. If different meta-atoms with desired phase distributions (i.e., \( \phi_{xi}^{+/-}(x, y) \) and \( \phi_{yi}^{+/-}(x, y) \) for reflection or transmission geometry, \( \phi_{xi}(x, y) \) and \( \phi_{yi}(x, y) \) for full-space metasurfaces) can be optimized, we can thus design metadevices/metasurfaces with pre-determined bifunctionalities with very high efficiencies.

We then describe another key factor to design multi-functional metasurfaces by suppressing the polarization crosstalk [61]. For an arbitrary anisotropic metasurface under the Cartesian coordinate system, we require four variables to describe the phase gradients \( \xi_x(x), \xi_y(x), \xi_x(y), \) and \( \xi_y(y) \) along different directions under different polarizations,

\[
\begin{bmatrix}
\xi_x(x) & \xi_y(x) \\
\xi_x(y) & \xi_y(y)
\end{bmatrix} = \begin{bmatrix}
\frac{\delta \phi_x(x, y)}{\delta x} & \frac{\delta \phi_y(x, y)}{\delta y} \\
\frac{\delta \phi_x(x, y)}{\delta x} & \frac{\delta \phi_y(x, y)}{\delta y}
\end{bmatrix}.
\]

(3.1)

Here, \( x \) or \( y \) in the subscript of \( \xi_x(x), \xi_y(x), \xi_x(y), \) and \( \xi_y(y) \) denotes the gradient direction, whereas that in the bracket represents the polarization direction. We thus have four degrees of freedom to describe and design anisotropic metasurface. According to the generalized Snell's law, the transverse \((k_x, k_y)\) and longitudinal \((k_z)\) wave vectors of the EM wave scattered by the metasurface (shined by a normally incident EM wave) are given by

\[
\begin{align*}
k_x(x/y) &= \xi_x(x/y) \\
k_y(x/y) &= \xi_y(x/y) \\
k_z(x/y) &= \sqrt{k_0^2 - k_x^2(x/y) - k_y^2(x/y)}.
\end{align*}
\]

(3.2)

Equation (3.2) shows that the wave-vector of the scattered EM wave can be controlled by both the incident polarization and the related phase gradient. These expanded freedoms are extremely helpful to achieve diversified EM characteristics. In practice, one typically obtains the
3.2 REFLECTION-GEOMETRY REALIZATIONS

The versatile beam-control metadevices that we designed are shown in Fig. 3.1. Two proof-of-concept metadevices, each combining two distinct complex functionalities including steered-beam, focused-beam, and multi-beam directional emissions. In both cases, the complicated phase profiles for two distinct functionalities require 2D geometrical-parameter searching and thus our strategy can save lots of time in designing such devices. The flexibly controlled highly directive emissions with multifunctionalities have huge fascinations and prospects to conveniently integrate complex systems with low costs.
Here, we propose a strategy to exhibit nearly negligible polarization cross-talk, such that the four phase gradients can be independently designed. The proposed anisotropic meta-atom contains two identical composite metallic resonators and a continuous metal plate separated by two dielectric spacers (2.5 mm–thick F4B board with $\varepsilon_r = 2.65 + 0.001i$); see Fig. 3.2a. To diminish the polarization cross-talk and broaden the bandwidth, we purposely designed the metallic resonator to contain both a metallic cross and an external wire loop. These two structures resonate at two different frequencies. Since the meta-atom is electrically subwavelength (0.277λ at 10 GHz), the two resonant modes can be quantitatively described by an equivalent circuit model (CM) shown in Fig. 3.2b, where the lower and upper mode around $f_1$ and $f_2$ are physically modeled by a series resonant tank formed by $L_1$, $C_1$, $R_1$, and $L_2$, $C_2$, $R_2$, respectively. Here, $L$, $C$, and $R$ represent the effective inductance, capacitance, and resistance (absorption) of the circuit. Figure 3.2c compares the spectra of reflection phase and amplitude for the single-layer and double-layer meta-atoms based on finite-difference-time-domain (FDTD) calculations. In the single-layer case, two reflection dips are clearly observed around $f_1 = 6.12$ and $f_2 = 9.9$ GHz resulted from two magnetic resonant modes generated by the couplings between the cross and its surrounding loop with the metallic ground plane, evidenced by the reversed currents on metallic patterns and ground plane as shown in Fig. 3.2g. Cascading the two resonances appropriately can significantly enhance the working bandwidth. Full-wave simulations (lines) are in good agreement with the CM calculations (symbols). When adding another resonator to form a double-layer meta-atom, couplings between different layers split the two resonances into four (dashed lines in Fig. 3.2c), and thus the working bandwidth is further enhanced, providing us more freedoms to engineer the phase slope. As depicted in Fig. 3.2d, changing $l_y$ from 0.5–3.65 mm leads to a large phase variation $\varphi_y$ of near 380° (full 360° cover), while changing $l_x$ has nearly no effects (37° phase shift of $\varphi_y$) on the spectra. The latter is highly desired indicating that the $y$-polarized response of our meta-atom is only sensitive to $l_y$ but is very insensitive to $l_x$. Symmetry consideration implies that the same conclusion can be drawn if we interchange the indexes $x$ and $y$.

In contrast, the polarization cross-talk effect is strongly enhanced if we remove the external wire loop from the resonator. As shown in Fig. 3.2e, in such a case the maximum variation of $\varphi_y$ is only 161° due to changing $l_x$ but can be as high as 83° due to changing $l_y$. Obviously, adding an external wire loop can significantly degrade the polarization cross-talk effects. The underlying physics of such an intriguing phenomenon can be understood by checking the field distributions on the cross-bar layers for the resonant modes associated with the $\vec{E} || \hat{y}$ polarization in two different meta-atoms, as shown in Fig. 3.2g. Due to the screening effect of the surrounding wire loop, the excited EM field is more strongly localized to the vicinities of the cross. In particular, the loop-bar coupling generates electric currents on the loop which significantly counteract the currents induced on the $x$-oriented bar, thereby making the mode rather insensitive to the parameter $l_x$. In contrast, non-negligible currents always exist on the $x$-oriented bar in the cross-only meta-atom even for the mode associated with the $\vec{E} || \hat{y}$ po-
3.2. REFLECTION-GEOMETRY REALIZATIONS

Figure 3.2: Illustration of the anisotropic meta-atoms without polarization cross-talk. (a) Topology of the dual-layer and single-layer anisotropic meta-atoms using composite crossbar and cross loop. (b) Illustration of geometrical parameters and equivalent circuit model. (c) Reflection coefficients of the single-layer and dual-layer meta-atoms in broad frequency spectrum, the circuit parameters are retrieved as $L_1 = 10$ nH, $C_1 = 0.05$ pF, $L_2 = 0.675$ nH, $C_2 = 0.108$ pF, $R_1 = 2.5$ Ω, $R_2 = 0.31$ Ω, $Z_c = 285.8$ Ω, and $h_o = 29.8^\circ$. Reflection coefficients of the dual-layer meta-atom (d) with and (e) without external wire loop in cases of different $l_x$ and $l_y$. (f) Reflection coefficients of the dual-layer meta-atoms as a function of $l_y$ at different frequencies of 9, 9.5, 10, and 10.5 GHz when $l_x = 2$ mm. The residual geometrical parameters are $p_x = p_y = 8.3$ mm, $r_x = r_y = 8.1$ mm, $l_x = l_y = 3.65$ mm, $d_1 = d_2 = 0.25$ mm, and $w = 1$ mm. All results are calculated under the excitation of $y$-polarized incident waves. (g) Current distributions on metallic patterns of the cross-only (left and middle panel), and cross-loop dual-layer meta-atoms (right panel). In FDTD calculation of reflection magnitudes/phases of meta-atoms, we studied a unit cell containing a single meta-atom with periodic conditions applied at its four boundaries to mimic an infinite array, and a floquet port assigned at a distance 15 mm away from the $x$-$y$ plane where the meta-atom is placed.
larization, generating the polarization cross-talk. Moreover, it is advisable to select a region far from the resonances to design our meta-atom with highly suppressed polarization cross-talk, as shown by the grey region of Fig. 3.2d. With the criterion to design our meta-atom known, we now show the bandwidth performance of the meta-atom. As illustrated in Fig. 3.2f, the reflection magnitude remains stable and is larger than 0.97 as \( l_y \) varies within 0.5–3.65 mm at 4 representative frequencies, indicating a satisfactory amplitude uniformity. More importantly, the four phase curves are almost parallel with each other and all exhibit good linear dependences on \( l_y \) in a large parameter region. One may easily expect that our meta-atom can work well in all frequencies lying in 9–10.5 GHz, where a full 360° phase coverage and near-unity magnitude can be simultaneously obtained by varying \( l_y \).

Further calculations indicate that the decrease of bar-width \( w \) improves the polarization cross-talk property but weakens the capability of phase accumulation, see Fig. 3.3a, where the reflection coefficient of our meta-atom changes as a function of its and \( l_x \). Again, the minimum and maximum values of \( l_x \) are set as \( w/2 \) and 3.65 mm, while \( l_y \) is fixed as 3.65 mm. Meanwhile, the resonant mode undergoes a slight red shift as \( w \) increases from 1 to 3 mm in the case of \( l_x = 3.65 \) mm. Therefore, increasing \( w \) deteriorates the irrelevance of \( l_x \) on \( \xi_x(y) \) and \( \xi_y(x) \) and that of \( l_y \) on \( \xi_x(x) \) and \( \xi_y(y) \), which is unfavorable for our design. However, further calculations indicate that the phase accumulation reduces when \( w \) is narrowed. For example, the phase difference as \( l_y \) changes from \( w/2 \) to 3.65 mm is 365° at 10 GHz for \( w = 0.5 \) mm, corresponding to 15° reduction relative to the case \( w = 1 \) mm. This is crucial for a large-array design since otherwise more layers should be added to guarantee the desired phase coverage and desirable polarization irrelevance, which are unfavorable to achieve low profile and high performance of devices. Balancing the two facts, we finally select a moderate value for \( w(w = 1 \) mm) in all designs. As shown in Fig. 3.3b, the phase is nearly a constant in the frequency regime 8–13 GHz when \( l_x \) increases from 0.5 to 3.65 mm, reinforcing that our meta-atom exhibits weak polarization cross-talking. The \( l_x \)-induced phase variation becomes non-negligible only at frequencies around 8.2 and 10.6 GHz where the two resonances are located and thus phase varies sharply. Above results indicate that it is advisable to select a region between the two highest resonances occurred when \( l_x = 0.5, l_y = 3.65 \) mm and when \( l_x = l_y = 3.65 \) mm, as shown by the grey region in Fig. 3.2d.

Before the formal design of the beam-control metadevices, we developed a general design methodology for any bifunctional devices under the framework of negligible polarization cross-talk. The design procedures mainly lie in four steps.

1. Design a subwavelength meta-atom with desirable polarization irrelevance and full 360° phase coverage within near-unity reflection amplitude and determine the basic structure parameters including periodicity \( p_x \) and \( p_y \). The primary criterion as set previously is to decorrelate the variation of \( l_y \) with \( \xi_x(x) \) and \( \xi_y(x) \) and that of \( l_x \) with \( \xi_x(y) \) and \( \xi_y(y) \).

2. Determine the necessary aperture phase and amplitude distributions according to the target hybrid functionalities under two orthogonal polarizations. In this particular design,
three sets of phase gradients are involved, i.e., the linear phase gradient for beam steering, the parabolic phase gradient for focusing (single pencil beam) and the hyperbola one for multiple pencil beams. For linear or parabolic phase gradient, the 2D phase distribution along x or y direction can be theoretically synthesized. For the hyperbola gradient, it cannot be directly obtained through analytical equations but need cautious optimization through alternating projection method (APM) to achieve extremely low sidelobes.

The main procedure of quad-beam synthesis using APM is to search for the intersection between the set of possible radiation patterns (set $A$) of a metasurface and that of target patterns with idealized performance (set $B$), based on closed-loop iterative optimizations $[147]$. The tangential components of the EM field emitted from a metasurface is the sum of waves radiated from different meta-atoms,

$$A \equiv \left\{ T : T(u, v) = \sum_{(m,n) \in I} a_{m,n} e^{jk(P^x_{m,n} u + P^y_{m,n} v)} \right\}. \quad (3.3)$$

Here, $I$ is the set of positions of all elements, $u = \sin \theta \cos \varphi$ and $v = \sin \theta \sin \varphi$ are the angular coordinates, $P^x_{m,n}$ and $P^y_{m,n}$ are positions of specific meta-atom along $x$ and $y$ direction, respectively, and $a_{m,n}$ denotes the contribution from the meta-atom located at the position citation $(m,n)$, determined by both the excitation field and the response (reflection amplitude and phase) of the meta-atom itself. The target pattern requirements are specified by two masks, i.e., the multiple pencil beams with uniform amplitude and high gain; and low sidelobes with negligible radiations relative to the peak value. In the first mask, the $-3\,\text{dB}$ beamwidth and each main beam of target patterns are characterized by the lower- and upper-bound values $$(M_L = $$
In the second mask, we define another upper bound $M'_U$ at certain elevation angle $\theta$. To minimize the side-lobe level, we require emitted fields in the side-lobe region must fulfill the following requirement:

$$B \equiv \{ T : |T(u, v)| = M'_U \}.$$  

(3.5)

The iterative optimization is considered to be converged and will be terminated when the cost function $T_{adp}$ reaches a stable value. In this particular design, $M'_U$ is restricted as an achievable value of $-30$ dB and the radiation pattern of the feed horn is modeled as $\cos^q(\theta)$ with $q = 8.6$,

$$T_{adp} = \sum_{u^2+v^2 \leq 1} \sum (|T(u, v)| - M'_U)^2.$$  

(3.6)

The synthesis consists of projecting the radiation patterns from set $A$ to set $B$, and projecting the patterns back to the aperture magnitude and phase distribution (inverse Fourier Transform (FFT) algorithms). In the former case, the radiation patterns are rectified progressively until both sets are in good proximity, whereas in the latter case the phase and amplitude of elements across the aperture are dynamically renewed and finally reach the optimum distribution. In the reflective scheme, the quad-beam metasurface design is related only to phase synthesis since the element amplitude is determined by aperture size and illumination. Before the phase optimization, one should predetermine some initial parameters such as feed position $F$ relative to metasurface, operation frequency $f_0$, aperture size $D$ and element number $N = D/p$, elevation angles $\theta$ and azimuth angles $\varphi$ that defining beam directions.

3. Choose an optimum strategy to cover the complete phase circle and obtain the phase-parameter database by FDTD parametric analyses. To guarantee sufficient precision, numerical interpolation is commonly adopted for available phase data with a mass of samples.

4. Determine the final metasurface by conducting a geometrical mapping process according to available phase distributions under two orthogonal polarizations based on a root-finding algorithm and phase-parameter database as shown in Fig. 3.2f. Thanks to the polarization irrelevance of the meta-atom, the geometrical parameters $l_x$ and $l_y$ can be separately determined by two polarization-dependent phase profiles $\varphi_x(x, y)$ and $\varphi_y(x, y)$, respectively.

Following above design procedures, we now employ the proposed anisotropic meta-atom to design the first versatile beam-control metadevice (denoted as sample I) to realize high-gain focused-beam and quad-beam emissions, triggered respectively, by $x$-polarized and $y$-polarized free-space excitations. As is shown in Figs. 3.4 and 3.5a, the metadevice is composed of a bifunctional metasurface I fed by a conical horn for excitation of both $x$ and $y$-polarized incident