Polarization insensitive all-dielectric metasurfaces for the ultraviolet domain

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Abstract: In recent years, metasurfaces have provided a tempting path to replace conventional optical components where an abrupt phase change is imposed on an incident wave using a periodic array of unit cells. Till date, highly efficient dielectric metasurfaces have been demonstrated in infrared and visible domains. However, due to the lower bandgap of typical dielectric materials, such metasurfaces present strong absorption in the ultraviolet (UV) domain, and thus, hamper their realization at shorter wavelengths. In this paper, we utilize a large bandgap dielectric material, niobium pentoxide (Nb2O5), to construct an ultra-thin and compact transmission-type metasurface that manipulates the phase of an incident wave using an array of Nb2O5 nano-cylinder. By the virtue of numerical optimization, complete 2π phase coverage along with the high transmission efficiency (around 88.5%) is achieved at 355nm. Such efficient control over the phase of the incident wave enabled us to realize the polarization insensitive self-accelerating parabolic, reciprocal, and logarithmic Airy beams (ABs) generating metasurfaces with the efficiency of 70%, 72% and 77%, respectively. In addition to this, we also demonstrate auto focusing Airy optical vortex (AFAOV) generators where the metasurfaces are designed to combine the phase profiles of an abruptly focusing Airy (AFA) beam and that of spiral phase plate (SPP). The AFAOV is generated with efficiency of 70% (for l = 3) and 72% (for l = 5).

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1. Introduction

The modern-day optical technologies aim to compact the physical dimensions of optical systems and integrate several chips. The conventional optical components are mainly depended on material intrinsic property to realize the desired functionality, resulting in the bulky optical devices. For instance, the optical lenses developed from the propagation of light through an optical medium over a distance much larger than incident wavelength for phase accumulation [1–3]. Contrary to conventional optical devices, metasurfaces (2D metamaterials) that are composed of periodic array of nano-scatterers (also known as unit cell) with subwavelength spatial resolution, provide the feasible esplanade to address issues offered by bulky optical devices due to their ability to manipulate the electromagnetic waves characteristics (amplitude, phase, and polarization) at will. This feature of metasurfaces makes them suitable for photonic integrated circuits and mass production. Based on metasurfaces, recently, many flat optical devices have been designed and realized including absorbers [4,5], holography [6–8], optical vortex generation [7,9–11], Bessel beams [12,13], self-accelerating beams [14,15], beam shaping [16–18] and so on.

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In earlier work, metallic nano-scatterer based transmission-type metasurfaces have shown better response from terahertz to near-IR [8,19–24]. However, due to electron-electron and electron-phonon scattering, the metallic metasurfaces encounter substantial ohmic losses, and temperature instability, causing a reduction in transmission efficiency in visible to UV domain, which is the region of interest for many potential applications (for example, bio-sensing, photolithography, and imaging applications) [25]. Recently, Aluminum (Al) based metasurfaces have shown promising responses at shorter wavelengths, but they undergo performance degradation due to oxidation [26]. To circumvent these limitations, high refractive indexed dielectric materials are considered as promising candidates to construct the lossless, and highly efficient metasurfaces at spectrum of interest [27]. To date, most of the research is focused on infrared and visible domains. Silicon-based metasurfaces have shown the transmission efficiency of >90% at infrared wavelengths [28], while amorphous silicon hydrogenated (a-Si:H) [11,29], titanium oxide (TiO$_2$) [30], gallium nitride (GaN) [31], and silicon nitride (Si$_3$N$_4$) [32] exhibit exceptional performance in the visible domain. However, these materials possess a small bandgap at UV range, thus render very low transmission efficiency [33,34]. Furthermore, UV transparent material such as CaF$_2$, MgF$_2$, and SiO$_2$ have low refractive indices present significant challenges in design and fabrication [33].

Consequently, we present highly efficient transmission-type all-dielectric metasurfaces employing niobium pentoxide (Nb$_2$O$_5$) material having the bandgap of 3.65 eV, which is significantly larger than other high indexed materials such as Si (1.1 eV) and TiO$_2$ (3.2 eV) [34]. Due to this intriguing feature, Nb$_2$O$_5$ exhibit a broader transparency window (covering the UV, Visible and Infrared) [35]. In this article, the manipulation of phase of impinging wave is performed using Nb$_2$O$_5$ based nano-cylinders. The cylindrical geometry of the unit cell is opted because of its insensitivity to polarization of incident wave [11,36]. The radius of nano-cylinder is varied to attain the complete $2\pi$ phase control of incident wave with high transmission efficiency (around 88.5%) at the working wavelength of 355nm (UV domain). Such efficient control facilitated us to realize the captivating phenomenon of self-accelerating parabolic, reciprocal, and logarithmic Airy beams (ABs) generation. The similar kind of work is published in [37] where the authors designed geometric phased based catenary-shaped plasmonic metasurfaces which require only circularly polarized incidence. Here, polarization insensitive ABs generating metasurfaces are presented with relatively high efficiency. Furthermore, we also demonstrate the autofocusing Airy optical vortex (AFAOV) generating multifunctional metasurfaces where phase profile of spiral phase plate (SPP) is integrated with that of abruptly focusing Airy (AFA) beam. We expect that this work would encourage establishment ultra-thin nano-photonic platform for bio-sensing, particle manipulation, and beam shaping applications.

2. Materials and methods

In order to realize the phase modulated metasurfaces, the first step is to achieve the $[0 - 2\pi]$ phase coverage through parametric optimization of unit cell while maintaining the maximum transmission efficiency. To accomplish this, Nb$_2$O$_5$ based nano-cylinder is patterned on SiO$_2$ substrate (the unit cell), as shown in Fig. 1(a). Here, $R$ represents the radius and $P$ periodicity while $H$ is the height of nano-cylinder. The Finite Difference Time Domain (FDTD) Numerical Method is employed for the optimization of Nb$_2$O$_5$ nano-cylinder at the working wavelength of 355 nm. The unit cell is subjected to perfectly matched layer (PML) boundaries in direction of propagation ($z$) and periodic boundaries in x-y direction. To acquire $2\pi$ phase control and maintain the high transmission efficiency, the periodicity ($P$) and radius ($R$) of nano-cylinders are swept with the optimal height ($H = 430$nm). The sweep results are depicted in Figs. 1(c) and 1(d). Here, it can be seen that the range of $R$ varying from 30 nm to 90 nm and $P$ of 182 nm (as indicated by the white dashed line) are an optimized choice. The average transmission efficiency of around 88.5% along with $2\pi$ phase coverage is attained. The transmission efficiency
and corresponding phase profile as a function of radius are illustrated in Figs. 1(e) and 1(f), respectively.

**Fig. 1. Unit cell optimization.** (a) Schematic of \(\text{Nb}_2\text{O}_5\) nano-cylinder on SiO\(_2\) substrate. Here parameters \(P\), \(H\), and \(R\) are the periodicity, height, and radius of the unit cell, respectively. (b) Step-indexed waveguide model of \(\text{Nb}_2\text{O}_5\) nano-cylinder. \(\text{Nb}_2\text{O}_5\) is considered as the core material while air (surrounding medium) represents the cladding. (c) Transmission efficiency and (d) Phase maps for radius versus periodicity at wavelength of 355 nm. The white dashed lines indicate the region of maximum transmission efficiency along with complete \(2\pi\) phase coverage. (e) Transmission efficiency versus radius at fixed periodicity of 182 nm. The average transmission efficiency of 88.5\% is achieved. (f) The comparison between phase profile (solid purple line) obtained through FDTD and phase profile (solid pink line) obtained through step indexed waveguide model as function of radius (varying from 30 nm to 90 nm).

The underlying physics of acquiring the specific phase profile via \(\text{Nb}_2\text{O}_5\) nano-cylinder can be well explained by wave guiding effect [36]. According to wave guiding effect, the phase yield by nano-cylinder with specific radius can be calculated in terms of effective refractive index \((n_{\text{eff}})\) with the help of the following relation:

\[
\Psi = \frac{2\pi}{\lambda} n_{\text{eff}} H
\]

where, \(H\) is the height of nano-cylinder and \(n_{\text{eff}}\) is the effective index of fundamental mode \((HE_{11})\) while \(\lambda\) is the operating wavelength. The \(n_{\text{eff}}\) can be computed through step-indexed waveguide model [38]. In which, \(\text{Nb}_2\text{O}_5\) nano-cylinder acts a core with refractive index \((n_{\text{core}})\) and surrounding medium (air) as cladding with refractive index \(n_{\text{clad}}\) (shown in Fig. 1(b)). As the radius of nano-cylinder is varied, the effective refractive index of fundamental mode is changed. Figure 1(f) shows that the phase profile calculated by step indexed waveguide model is in agreement with the one calculated through FDTD simulation. The agreement seems better.
for larger radii where the confinement of mode increases. Furthermore, periodic boundary conditions in FDTD also introduce deviation in mode profile which is dominant for smaller radii, thus indicating the reason behind the difference between two phase profiles.

Furthermore, it is necessitated that for high contrast dielectric metasurfaces, the interaction between the unit cells should be negligible and scattering of incident light is purely dominated by wave guiding effect. To verify this, the numerical simulations for three different radii (50 nm, 60 nm, and 70 nm) are performed to investigate the near field distributions. In Fig. 2, the top (first row) and side (second row) views of magnetic energy densities (MEDs) inside arrays of nano-cylinders with different radii are shown. It can be observed that most of the incident light is concentrated inside the nano-cylinders and have negligible coupling with neighboring nano-cylinders. Therefore, transmission phase and efficiency of periodic array of unit cells can be considered as the individual response of each unit cell [39–41].

![Fig. 2. Near field distribution of periodic arrays of unit cell.](image)

3. Results and discussion

3.1. Polarization insensitive Airy beam generators

To proof the concept of phase modulation, here, we demonstrate the polarisation insensitive AB generating metasurfaces. According to the geometric construction of arbitrary optical caustics, the ABs along the convex trajectories can be produced by directly employing the spatial phase profile on an impinging beam [42,43]. In this regard, the phase profile for parabolic 1D AB as depicted in Fig. 3(a) is implemented and can be expressed as follows:

$$\Psi(x) = -\frac{4}{3}(a)^{2}k(x)^{2}$$  \hspace{1cm} (2)

where, ‘a’ is the coefficient of acceleration associated with curved trajectory of parabolic AB (here, a = 0.014µm⁻¹), and ‘k’ is the wave number. The spatial distribution of the phase is materialized by adjusting the radii of Nb₂O₅ nano-cylinders (obtained from Fig. 1(f)) placed at each coordinate point. Hence, 11µm x 11µm metasurface, embedding the parabolic phase profile is designed and simulated.

The full-wave numerical simulation of our designed metasurface is accomplished via FDTD method. The metasurface is subjected to Perfectly Matched Layered (PML) boundary condition in all directions (x, y, and z). The x-polarised plane wave in impinged onto the metasurface and resultant outgoing electric field is recorded by placing field monitor in x-y plane. Figure 3(b)
parabolic nature of our AB, analytically calculated \((x^2 = az^2)\) and simulated propagation trajectory of main lobe is plotted in Fig. 3(c). Here, we can see the good match between analytically calculated and simulated results. However, it is believed that the small deviation is due to the fact that discrete number of unit cells are approximating continuous phase function.

In addition to parabolic AB, here we also demonstrate the metasurfaces, capable of generating ABs that follow the reciprocal \((x = a/z)\) and natural logarithmic \((x = a \ln(bz))\) caustic trajectory. The corresponding spatial distribution of phase profiles as depicted in Figs. 3(d) and 3(g) respectively, can be expressed as:

\[
\Psi(x) = kx^3/a^2, \quad (3)
\]

and

\[
\Psi(x) = -k a^2 b k (1 - \frac{1}{\sqrt{y}}), \quad (4)
\]

**Fig. 3. Polarisation Insensitive Airy beams generation.** (a), (d), and (g) show the Spatial phase distributions of parabolic AB, reciprocal AB, and logarithmic AB, respectively. (b), (e) and (h) represent the corresponding simulated E-field intensity distribution imaged in x-z plane. (c), (f), and (i) demonstrate the comparison between analytically calculated and simulated propagation trajectories of main lobes of parabolic AB, reciprocal AB, and logarithmic AB, respectively.
illustrates the simulated electric field (E-field) distribution showing the self-bending and self-accelerating nature of main lobe of parabolic AB. To further verify the parabolic nature of our AB, analytically calculated \( x_d = az^2 \) and simulated propagation trajectory of main lobe is plotted in Fig. 3(c). Here, we can see the good match between analytically calculated and simulated results. However, it is believed that the small deviation is due to the fact that discrete number of unit cells are approximating continuous phase function.

In addition to parabolic AB, here, we also demonstrate the metasurfaces, capable of generating ABs that follow the reciprocal \( x = a_1/z \) and natural logarithmic \( x = a_2 \ln(bz) \) caustic trajectory. The corresponding spatial distribution of phase profiles as depicted in Figs. 3(d) and 3(g) respectively, can be expressed as:

\[
\Psi_{\text{rec}}(x) = \frac{kx^3}{3a_1},
\]

and

\[
\Psi_{\text{ln}}(x) = -e^{-1}a_2^2 bk \left(1 - e^{-\frac{a_2}{bk}}\right).
\]

Here, \( a_1 = 60 \mu m^{-1}, a_2 = 4 \mu m^{-1}, b = 0.1 \mu m^{-1} \) are chosen as coefficients of acceleration. Figures 3(e) and 3(h) illustrates the electric field distribution of reciprocal and natural logarithmic ABs. To confirm the desired caustic, the comparison between the analytically calculated and simulated propagation trajectories of main lobe are plotted in Figs. 3(f) and 3(i). It can be seen that the simulated propagation trajectories validate the analytical predictions with little deviation. The transmission efficiency of 70% (parabolic), 72% (reciprocal), and 77% (logarithmic) is achieved which seems better compared to recently reported work [37].

Furthermore, to reveal the polarization insensitive feature of our Airy beam generator, we simulate parabolic AB generating metasurface by impinging incident wave with different polarizations. The simulated results (in x-z plane) are demonstrated in Figs. 4(a)–4(c) where the parabolic Airy beams are generated for y-polarized, right circular polarized (RCP), and left circular polarized incidences (LCP).

![Fig. 4. Polarisation insensitivity test. Simulated E-field distribution of parabolic AB under illumination of (a) y-polarisation (b) RCP, and (c) LCP at operational wavelength of 355 nm.](image)

3.2. Auto focusing Airy optical vortex (AFAOV) generators

In this section, we propose the phase modulation based multifunctional metasurfaces capable of generating AFAOVs. To realize such metasurfaces the phase profiles of Abruptly focusing Airy (AFA) and Spiral Phase Plate (SPP) are merged together. The resultant relation for required
phase distribution can be expressed as follows:

\[ \Psi = -\frac{4}{3}(a)^{\frac{1}{2}}k(r-r_o)^{\frac{1}{2}} + l\theta. \] (5)

The Eq. (5) can be envisioned as the radial version of Eq. (2) with an additional phase of SPP. Here, ‘k’ is the wave number, ‘a’ is coefficient of acceleration, ‘r_o’ is the transparent region, ‘l’ is the topological charge, and \( \theta \) is the azimuthal angle. Where the focal length can be defined as [44]:

\[ f = \sqrt{r_o - a} \] (6)

Here, two metasurfaces for topological charge \( l = 3 \) and \( l = 5 \) are designed with focal length of 11\( \mu \)m. The radius ‘r’ of both devices is kept 5.5\( \mu \)m with \( r_o = 0.91\mu \)m as a transparent region, and 

\[ a = 0.00735\mu m^{-0.5}. \]

Figures 5(a) and 5(b) shows the spatial distribution \( \text{Nb}_2\text{O}_5 \) nano-cylinder distribution for \( l = 3 \) and 5, respectively. Under the \( x \)-polarised incidence, the FDTD numerical simulations of AFAOV generating metasurfaces are performed by applying Perfectly Matched Layered (PML) boundary conditions in \( x, y, \) and \( z \) dimensions. The annular openings in Figs. 5(c) and 5(d) shows the cross-sectional intensities for \( l = 3 \) and 5 respectively, recorded by placing E-field monitor at focal plane. It is observed that radius of annular opening increases as the topological charge increases followed by the increase in number of spirals in phase pattern, portrayed in Figs. 5(e) and 5(f). The simulated focusing efficiencies are 72\% (for \( l = 3 \)) and 70\% (for \( l = 5 \)). These efficiencies are comparable to recently reported work [28].

**Fig. 5. Auto Foucsing Airy Optical Vortex Generation.** (a) and (b) Phase distribution of \( \text{Nb}_2\text{O}_5 \) nano-cylinder for (a) \( l = 3 \) and, (b) \( l = 5 \). (c) and (d) Simulated E-field intensity distribution in \( x-y \) plane for \( l = 3 \) and 5, respectively. These donut shaped annular openings are imaged at focal plane \( (z = 11\mu m) \). (e) and (f) show their corresponding phase patterns.
4. Conclusion

In conclusion, all-dielectric metasurfaces in UV domain are proposed by using niobium pentoxide (Nb$_2$O$_5$). Periodic arrangement of optimized Nb$_2$O$_5$ nano-cylinder enabled us to manipulate the phase of incident wave with high transmission efficiency of 88.5%. Based on this, highly efficient polarisation insensitive AB generating metasurfaces are present to convert the incident wave with arbitrary polarization into self-accelerating ABs (parabolic, reciprocal, and logarithmic) with efficiency from 70% – 77%. Furthermore, the self-bending nature of main lobes of ABs have shown good agreement with analytical calculation with slight deviation. This deviation is due to discrete phase distribution. In addition to this, we extended our approach to realize the AFAOV generating metasurfaces where phase profile of AFA and SPP is merged to generate highly concentrated AFAOV. Two metasurfaces for $l = 3$ and 5 are designed and simulated with focusing efficiency of 72% and 70%, respectively. We envision that our designed metasurfaces can be useful for micron scale particle manipulation, optical tweezers, and bio-sensing.

Disclosures

The authors declare no conflicts of interest.

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