# Design of multi-wavelength dielectric metasurfaces using finite element software

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*This paper is dedicated to Padmashree Prof R S Sirohi*

Dielectric metasurfaces have great potential in compact optical systems. Most researchers use Finite Difference Time Domain (FDTD) based tools, such as Lumerical FDTD, to design and model meta-surfaces. In this paper, we explore the use of a Finite Element Method (FEM) based tool that may be more easily available, namely COMSOL Multiphysics software. A step-by-step design approach is presented to help researchers wanting to use metasurfaces for their work. Both monochromatic and two-wavelength system designs are explained in detail. In the former case, a cylindrical metasurface unit cell is simulated in COMSOL and the results are found to match with the results carried out using FDTD methods. Further, a spherical lens and an axicon or conical lens that works at two different wavelengths (1300 nm and 1550 nm) are designed. Their functionality is verified through simulation in COMSOL. In this design, coupled rectangular dielectric resonators are used as the unit cell structure. By implementing these specific optical functions, the use of COMSOL as a numerical tool in modelling dielectric metasurfaces is established.

**Keywords**: Dielectric metasurfaces, Multi-wavelength, COMSOL.

## 1 Introduction

Optical systems have long transited from simple light collection and focusing systems to ones that create complex light beams useful for imaging, optical particle trapping, microscopy and high-speed optical communication. The unique features of complex light beams were found to be useful especially to generate high resolution images from deeper tissues in medical diagnostics applications. Portable compact optical devices led to the need for shrinking of optical components without compromising performance or efficiency. Optical metasurfaces have emerged as an efficient flat optics solution, in this era of planar photonics. Dielectric metasurfaces, often defined as an array of subwavelength phase shifters have a prominent role in modern optics especially in realizing metalenses as they exhibit high transmission efficiency and unidirectional scattering [1]. A dielectric metasurface can support electric and magnetic resonant modes at the wavelengths of interest [2]. The primary goal of a metasurface is to impart a spatially varying phase to the incident light with unit cells of varying lateral dimensions spread across the metasurface [3]. Different resonator structures such as cylindrical disks [4,5], or antennas that are cross-shaped [6], V-shaped [7], nanofin-based [8,9], etc., have been deployed in realizing dielectric optical metasurfaces. Most of these metasurfaces are narrow-band and can be used in applications where a monochromatic source is used.

Multi-wavelength achromatic metasurfaces started gaining significance as they are useful for a wide range of applications such as colour imaging, displays, dispersion control, etc. Several design approaches such as spatial multiplexing of metasurface atoms [10], frequency selective meta-atoms [11], multiple meta-

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atoms per unit cell [12], etc have been presented to realize multiwavelength or broadband metasurfaces. The goal of a multiwavelength achromatic metalens is to achieve the same total accumulated phase for light of specific wavelengths travelling through the system. Dispersive phase compensation is the fundamental principle used by most researchers for designing achromatic metasurfaces. Since the phase accumulated by light due to propagation in air is wavelength dependent, the engineered metasurface capable of compensating for this dispersive phase has to be designed [12].

Lumerical FDTD is the EM field solver used by most researchers in designing metasurfaces. The design involves intensive FDTD computations to obtain the metasurface layout for the desired optical element. FDTD and FEM are inherently more suited to analyze arbitrary complex 3-D geometries as they discretize the entire object and background region. Although commercial FDTD solvers like Lumerical are very expensive; FEM based tools, like COMSOL Multiphysics (COMSOL), have surprisingly not been explored much by researchers in the design of metasurfaces. A paper that uses COMSOL presents the design of metasurfaces; simulating a plasmonic metalens with V-antennas as the meta-atom [13]. In addition to this, FDTD tools by default compute wideband solutions, even if the design is going to be used at a single wavelength. It should be noted that the wideband solutions of FDTD methods are not achromatic solutions. Even when designing elements for multiple wavelengths, frequency methods like FEM are better suited than time domain methods like FDTD [14]. It has been shown [15] that COMSOL yields results that are almost in perfect agreement with Mie's theory, for scattering cross sections, near field intensities, and far field patterns in the case of nano-spheres. In this paper, we investigate the competence of COMSOL as a software tool for simulating dielectric optical metasurfaces.

This paper is organized in two parts. The first part involves a comparison between COMSOL and Lumerical when designing a single wavelength dielectric metasurface for a specific application. The second part presents the simulation of a multi-wavelength dielectric metasurface using COMSOL. Two examples are taken, namely that of a cylindrical metalens and an axicon.

## 2 Design of dielectric metasurfaces for use at a single wavelength

The design of a metasurface involves three steps. The first step is to generate different meta-atom dimensions corresponding to different phase values. In this way, a phase lookup table can be created that provides a relationship between the size of a certain meta-atom and the phase it provides. The sizes should be such that a phase coverage 0 to $2\pi$ is achieved for the desired wavelength. The second step is to generate the target phase profile o (Qf the desired optical element. The final step is to generate the metasurface by replacing the target phase profile with the appropriate meta-atoms. A continuous target phase profile need not be realised as such but can be discretized into a different number of levels. The number of levels of discretization will determine the efficiency of the designed optical element. Converting a continuous phase profile into just 4 discrete phase levels will yield greater than 80 percent efficiency [16]. Figure 1 shows the conversion of a blazed grating into a 4-level metasurface. Similarly, any target phase profile can be converted to the desired number of discrete phase levels using the relevant meta-atoms.

The meta-atoms used for designing a metasurface can be of different shapes. A cylindrical meta-atom is a popular choice for realizing single wavelength optical elements due to its polarization insensitivity [4,5]. In applications that require full control of the wavefront, the different meta-atoms must provide a phase shift covering the entire range from 0 to $2\pi$ [7]. In dielectric metamaterials with high refractive index this complete phase coverage is obtained due to the overlap of electric and magnetic dipole resonances. Hence, silicon, which has a high refractive index in the visible and IR spectral regions is a popular choice for realising dielectric metasurfaces [1]. Once the shape and the material are decided, the next consideration is the dimensions of the structure. The major advantage of using a metasurface based optical element instead of a diffractive optical element is that in the former, structures with the same height can still provide different phase values. Thus, a highly efficient metasurface element can be fabricated with a single lithographic process. In order to achieve a phase shift from 0 to 2π, the radius of the cylinder of a meta-atom should be varied. Finding the phase shift imparted by cylinders of different radii is done by using numerical analysis methods like FDTD, FEM or Integral Equation Method (IEM). Along with the phase shift imparted by the meta-atom, the transmittance should also be considered to get the best efficiency. Using a numerical method, a phase lookup table is created by sweeping the radius of the cylinder over a large window. The lookup table will contain different radii that provide full phase coverage, while providing a good transmittance.

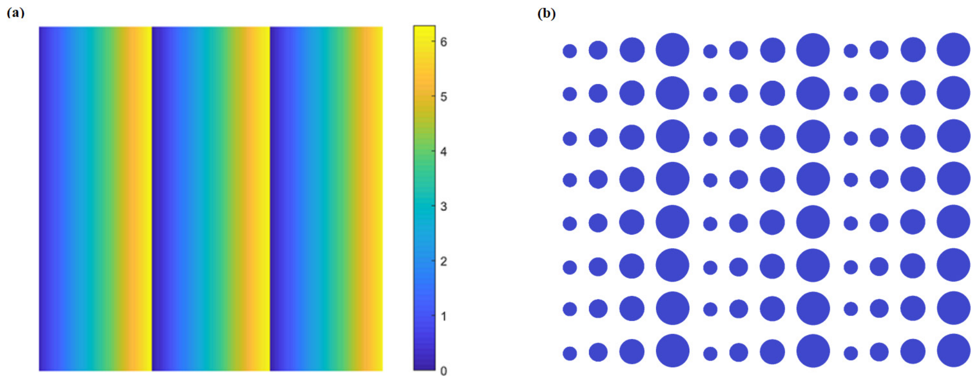


Fig 1. (a) Phase profile of a blazed grating (b) Conversion of continuous phase to four-level phase with respective unit cells replacing the phase profile.

### 3 Simulation of cylindrical meta-atoms using COMSOL

In the present work, we use COMSOL, which is based on FEM, for generating the phase lookup table. The main objective is to establish the competence of COMSOL for the analysis of these kinds of problems. Figure 2 (a) shows the meta-atom simulation in COMSOL. A silicon cylinder placed over a quartz substrate constitutes the meta-atom. To determine the phase shift and transmittance, a simple 2-port system

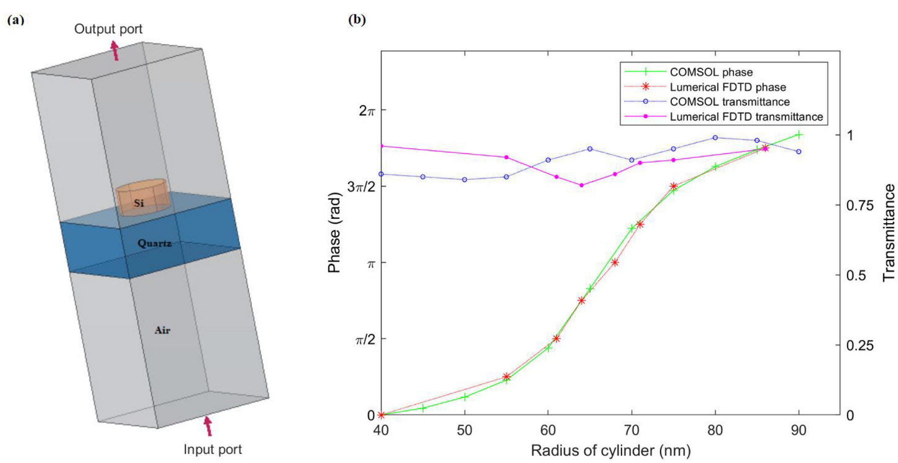


Fig 2. (a) Unit cell simulation model in COMSOL. Periodic boundary condition on all four faces and port boundary condition on top and bottom (b) COMSOL and Lumerical FDTD lookup data comparison: Phase of unit cell vs radius of cylinder at 633 nm wavelength.

with periodic boundary conditions at all four faces is considered. The port boundary conditions at the top and bottom ensures the absorbing boundary conditions. The ports are kept at a sufficient distance from the structure so that there is no evanescent field effect. An initial simulation solves the total accumulated phase at the output port without meta-atom in the model. Then the simulation is repeated after adding the meta-atom to the model. By using the data obtained in these two simulations, the phase shift imparted by the meta-atom alone is calculated. In each case, the transmittance value at the output port is also noted. The simulation is done for different radii using a parameter sweep and the phase lookup table is generated. A particular radius is chosen such that it imparts the required phase while giving a transmittance close to one.

Figure 2(b) shows simulation results in COMSOL compared with the results obtained using Lumerical FDTD. The results of Lumerical FDTD are from an earlier work [3]. It can be seen from the figure that the simulation results for the phase shifts imparted by the meta-atoms are perfectly matching. By implementing this simple design using COMSOL, we were able to validate that COMSOL could provide results similar to that of Lumerical FDTD. This result gives us confidence to proceed to more complex designs for multi-wavelength applications in COMSOL. The design of a multi-wavelength metalens using COMSOL is discussed in the next section.

## 4 Design and simulation of optical elements for multi-wavelength operation based on dielectric metasurfaces

Conventional metasurfaces are affected heavily by chromatic aberration [12,17,18]. A phase lookup table generated for a particular wavelength will not be suitable for another wavelength. One of the approaches to achieve achromatic behaviour is to compensate the phase accumulated by propagation through free space by the phase shift imparted by the meta-atom considering a particular functionality. This dispersive phase compensation technique is position dependent, as a meta-atom at a particular location needs to compensate for the phase accumulated at that location by each wavelength. Hence, it is not possible to generate a single-phase lookup table and replace the target phase profile with the corresponding meta-atom, as in case of the single wavelength. When designing for multi-wavelength use, the target phase function of the metasurface should be such that it compensates for the wavelength dependence of free space propagation [12]. To illustrate this in the design of a multi-wavelength element, we consider a cylindrical lens.

Example 1: Cylindrical Lens

The simulations are carried out for a 1-d element but can be extended to two dimensions, if necessary. The element is equivalent to that of a bulk refractive lens and the target phase function of the metasurface is given by Eq (1)

$$\phi_m(x, \lambda_i) = \frac{-2\pi}{\lambda_i}\sqrt{(x^2 + f^2)} - f \tag{1}$$

Here, $x$ is the spatial coordinate, $f$ is the focal length of the lens and $\lambda_i$ is the wavelength of interest. A cylindrical lens is considered here so that a 2D simulation in COMSOL can be done to implement the lens functionality. From the equation, it is clear that different wavelengths will have different target phases at any particular location. Figure 3(a) shows the variation of target phase with position for the wavelengths, 1300 nm and 1550 nm. The focal length of the lens is taken as 20 mm and the diameter of the lens is 600 μm. In order to realise a metalens that works at the desired wavelengths, an appropriate meta-atom that imparts the target phase shift at the particular location should be used. Cylindrical structures with one degree of freedom (e.g., radius) will not be suitable for this purpose, as with such meta-atoms it will not be possible to achieve the required phase values at each wavelength.

Alternatively, a coupled Rectangular Dielectric Resonator (RDR) could be used. These resonators were one of the earliest multiwavelength structures designed on the principle of dispersive phase compensation. In case of a coupled RDR, the unit cell will consist of two rectangular resonators separated by a gap. In a coupled RDR structure, unlike the cylindrical structure, the electric and magnetic dipole resonances do not overlap. Therefore, the phase shift imparted by these resonators varies only in the range of 0 to $\pi$. But the scattered field due to the dielectric resonators along with the diffracted field due to the slot in-between the resonators gives a larger phase variation in the total field which spans all four quadrants [12]. Figure 3(b) shows the coupled RDRs used for designing the metasurface. Compared to cylindrical structures, they have more degrees of freedom; namely the width of the resonators '$w_1$' and '$w_2$' and the gap '$g$' between the resonators. All of these can be varied to obtain the required phase shift and transmittance. Simulation is done only in 2D in order to reduce the computational cost.

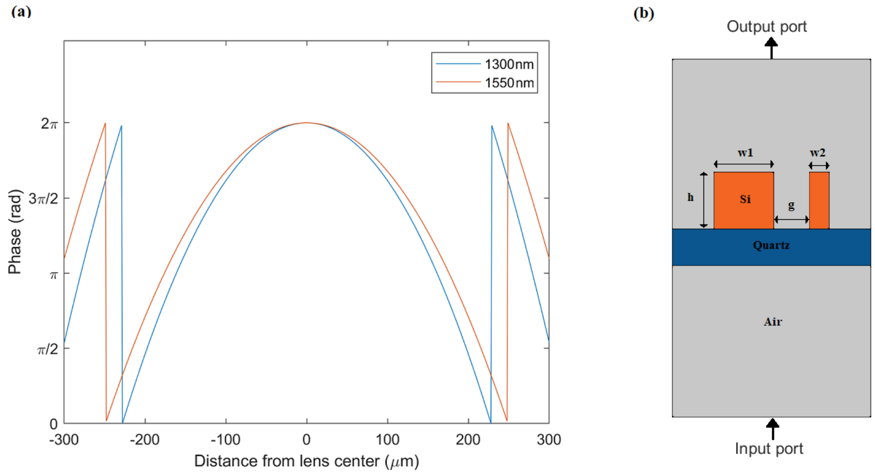


Fig 3. (a) Target phase function of a metalens at 1300 nm and 1550 nm (b) 2D model of multi-wavelength unit cell.

Finding the right geometry of the meta-atom that satisfies the required target phase value for both 1300 nm and 1550 nm is a difficult process. The phase shift and transmittance corresponding to a particular geometry is determined in a similar way as discussed in case of the single wavelength. In this case however, there are three parameters that can be varied and the number of different geometries possible are much higher. In our simulation, the parameters '$w_1$' and '$w_2$' are varied from 75 nm to 500 nm in steps of 25 nm and the gap '$g$' is varied from 0 nm to 500 nm in steps of 25 nm. It is also ensured that the size of the entire meta-atom does not exceed 1000 nm. The width of the meta-atom is, therefore, taken as 1000 nm and the height is fixed to 400nm. Sweeping the parameters in the above-mentioned ranges will yield about 4000 different geometries. The most suitable geometry that gives the required target phase at a particular location will implement the lens functionality. Such a geometry that satisfies both the wavelengths may not be available. Moreover, placing meta-atoms of different geometry in each unit position throughout the metasurface is not also feasible. In our design, we discretise the target phase function into different zones based on position. The meta-atom for each zone is chosen in such a way that it satisfies the average target phase value for both wavelengths at that particular zone. A sufficient tolerance of target phase value also has to be considered while choosing the meta-atom at a particular location. All these approximations will reduce the efficiency of the element, which is the cost paid for achieving the multi-wavelength functionality.

From the large data set obtained by sweeping the three parameters, a metalens of 600 µm diameter is constructed using suitable meta-atoms at each zone. Initial design is done in such a way that the geometries chosen suit the phase levels of 1550 nm alone. Then in the next stage, the design is optimised so that the element works for both 1550 nm and 1300 nm. After the meta-atoms are arranged in their suitable positions, the electric field in the near field region is evaluated by giving a plane wave as input to the entire metasurface. Then the Fresnel integral equation [19] is used to propagate this field to a distance of 20 mm, which is the focal plane of the lens designed. Table 1 shows the dimensions of the meta-atoms used for the first design along with the transmittance and phase values at each wavelength.

From Table 1, it can be seen that 4 different meta-atoms are used to discretise the phase function in the different positions of the lens. The geometries given in the table are specifically chosen for 1550 nm. In case of 1550 nm, the chosen geometries impart phase shifts that discretise the entire 0 to 2π phase range properly while providing good transmittance values. The data corresponding to 1300 nm indicates that the quality of discretisation is very poor. The transmittance values for 1300 nm are also not very good. Thus, it can be expected that the focusing at 1300 nm will be very poor compared to that of 1550 nm. This is evident from the results shown in Fig 4. In the next part of the design these geometries will be modified such that they impart phase shifts that reasonably discretise the target phase function at both wavelengths. The transmittance value at both wavelengths should also be taken into account while choosing the meta-atoms.

Table 1. Details of meta-atoms used for designing 1550 nm metalens (*maximum transmittance value is 1)

| Unit cell dimensions (nm) | | | $\lambda_1 = 1550$ nm | | $\lambda_2 = 1300$nm | |
|---|---|---|---|---|---|---|
| $w_1$ | $w_2$ | g | Transmittance* | Phase (degrees) | Transmittance* | Phase (degrees) |
| 250 | 200 | 475 | 0.68 | 342 | 0.13 | 289 |
| 100 | 175 | 175 | 0.65 | 250 | 0.66 | 276 |
| 125 | 250 | 350 | 0.65 | 164 | 0.43 | 295 |
| 125 | 300 | 100 | 0.41 | 80 | 0.24 | 307 |

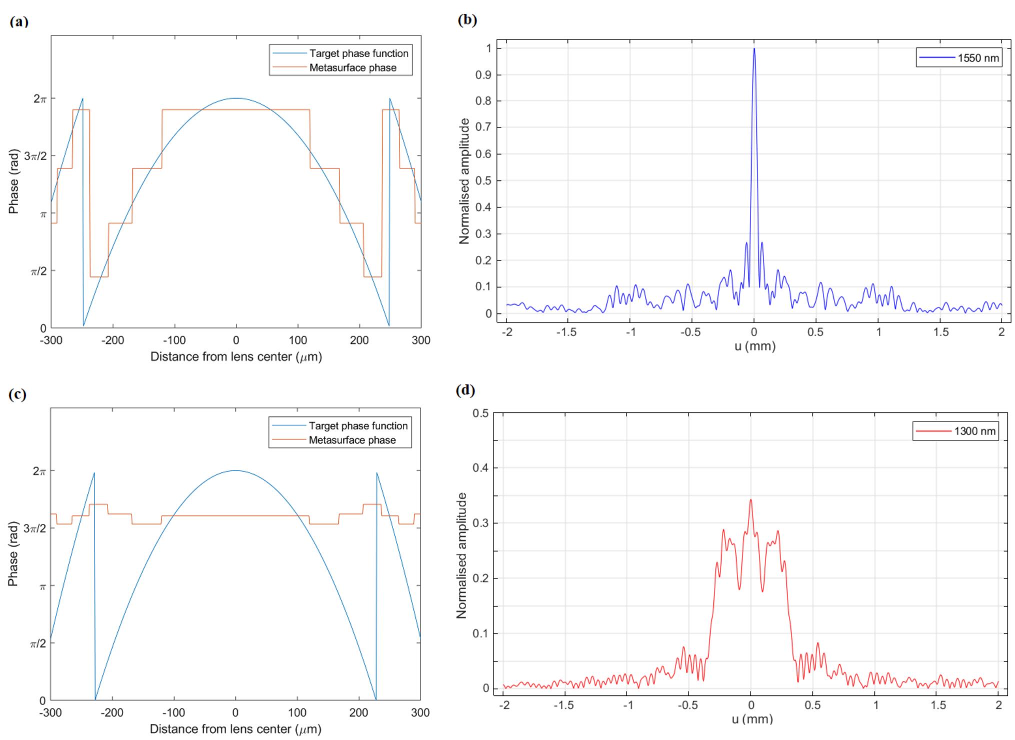


Fig 4. Metalens design suited for 1550 nm. (a) Target phase function of metalens and the achieved phase in the near field for 1550 nm (b) The beam obtained at the focal plane for 1550 nm (c) Target phase function of metalens and the achieved phase in the near field for 1300 nm (d) The beam obtained at the focal plane for 1300 nm.

Figure 4 shows the simulation results of the metalens designed specifically for 1550 nm. The target phase and the achieved phase in the near field region is given in Fig 4(a) & 4(c) for 1550 nm and 1300 nm, respectively. As expected, the focused beam (Fig 4(b)) obtained for 1550 nm is much better than that obtained at 1300 nm (Fig 4(d)). To improve the performance of the element at 1300 nm, the geometry of the metasurface has to be modified such that the element gives better discrete phase values and transmittance for 1300 nm, while simultaneously not causing much variation in the 1550 nm phase levels. Initially, suitable geometries from the dataset are chosen by setting a tolerance for both phase and transmittance. The metasurface is then modified using the new geometries and the phase achieved in the near field region is analysed. Fine tuning of the geometries is done so that the relative phase difference between different phase levels has not increased due to the tolerance applied.

Table 2 gives the details of the meta-atoms used in the design of metalens optimised for both 1300 nm and 1550 nm. Figure 5 shows the simulation results for this design. It can be seen from Fig 5(a) & 5(c)

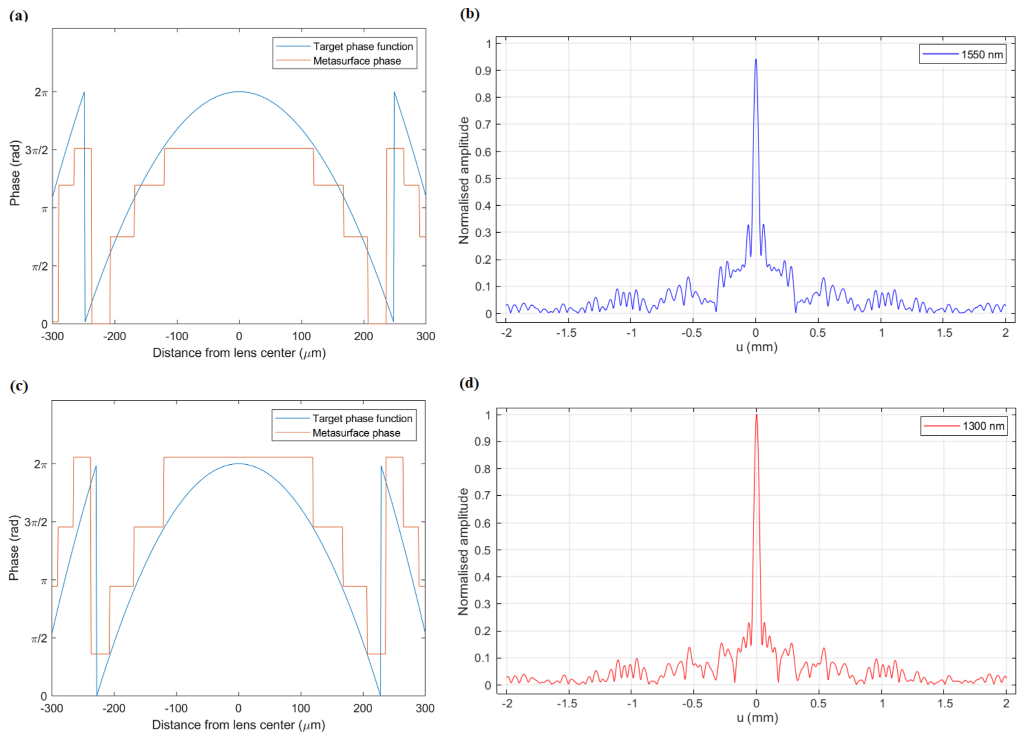


Fig 5. Metalens design optimised for both 1550 nm and 1300 nm. (a) Target phase function of metalens and the achieved phase in the near field for 1550 nm (b) The beam obtained at the focal plane for 1550 nm (c) Target phase function of metalens and the achieved phase in the near field for 1300 nm (d) The beam obtained at the focal plane for 1300 nm.

Table 2. Details of meta-atoms used for the design of metalens optimised for both 1300 nm and 1550 nm

| Unit cell dimensions (nm) | | | $\lambda_1 = 1550$ nm | | $\lambda_2 = 1300$nm | |
|---|---|---|---|---|---|---|
| $w_1$ | $w_2$ | $g$ | Transmittance | Phase(degrees) | Transmittance | Phase(degrees) |
| 500 | 325 | 150 | 0.59 | 272 | 0.56 | 370 |
| 125 | 150 | 300 | 0.80 | 215 | 0.61 | 262 |
| 75 | 75 | 425 | 0.82 | 135 | 0.90 | 170 |
| 200 | 225 | 0 | 0.76 | 0 | 0.41 | 65 |

that the discrete phase levels achieved from the metasurface are now suited for both wavelengths. This can also be seen from the focused beam in the Fig 5(b) & 5(d). It can be seen that in the process of improving the focusing of the lens for 1300 nm, the focusing at 1550 nm has deteriorated slightly. Again, this is an acceptable trade-off considering the improvement in the functionality at 1300 nm. It should be noted that in all these simulations only four phase levels are used, which limits the achievable quality as well.

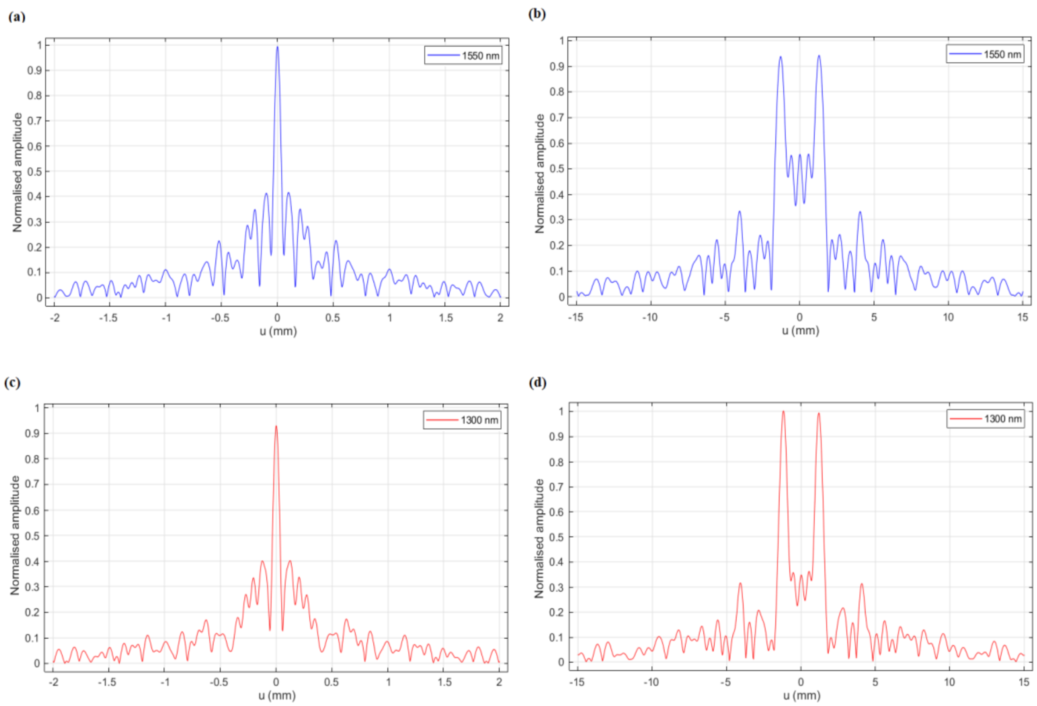


Fig 6. Simulation results of the field after the axicons designed at both wavelengths. (a) Bessel pattern obtained at a distance 28mm from the metasurface for 1550 nm (b) Two focused spots obtained at the far field for 1550 nm (c) Bessel pattern obtained at a distance 28mm from the metasurface for 1300 nm (d) Two focused spots obtained at the far field for 1300 nm.

Example 2: Axicons or Conical Lenses

The structure of a conical lens (axicon) is similar to the spherical lens except that its surface is in the shape of a cone. These elements have attracted much attention of late, due to the many important applications of Bessel beams that are generated by such elements [20]. As in the case of the spherical lens, only one spatial dimension is considered in this design to reduce the computation time. The target phase function of the metasurface for a 1-d axicon is given by the following equation.

$$\phi_{m1}(x, \lambda_i) = \frac{-2\pi}{\lambda_i} x \tan(\alpha) \tag{2}$$

where $x$ is the spatial coordinate, $\lambda_i$ is the wavelength of interest and $\alpha$ is the cone angle. When a plane wave is incident on an axicon, it will produce a Bessel pattern throughout the Depth of Focus (DOF) of the lens. At the far field, a ring pattern is formed. Since in this design, we are considering only one spatial dimension, two focused spots will be obtained at the far field. The DOF of the axicon is given by [21],

$$DOF = R / \tan(\propto) \tag{3}$$

where $R$ is the radius of the axicon. The radius of the axicon designed is 300 μm and the cone angle is 0.35° which yields a DOF of about 49 mm.

Figure 6 shows the simulation results obtained for the designed axicon. In case of Fig 6(a) and 6(c), the beam is propagated to a distance within the depth of focus of the axicon. The Bessel beam formed can be seen in these figures. In the second case, the beam is propagated to the far field region. The results are shown in Fig 6(b) and 6(d), where two peaks can be seen which correspond to the two focused spots. Again, it must be pointed out that the use of only 4 phase levels means that the entire phase range will not be discretized so as to perfectly match the desired phase. This limits the achievable quality of the final Bessel beam.

## 5 Conclusion

In this paper, we have presented the design flow for both a single and multi-wavelength dielectric metasurface. All results are validated using COMSOL as the design tool, rather than the more popular Lumerical FDTD software. The results clearly demonstrate that COMSOL, which is an FEM based design tool, performs as well as FDTD based design tools when used for designing dielectric metasurfaces. FEM-based approaches are inherently more suited for these kinds of applications and will require less computational cost. We believe this work will provide more confidence in using FEM based tools for designing metasurfaces.

We also designed multi-wavelength optical elements using coupled RDRs and successfully showed the functionality for two different wavelengths, 1300 nm and 1550 nm. The efficiency of the designed elements can be improved further by simulating more geometries or by using more complicated structures that could provide better phase coverage. Optimising the results for multiple wavelengths is currently done by a trial-and-error method. More advanced techniques need to be incorporated to reduce the time required for the optimisation process.

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