Plasmon-enhanced Optical Rotation in Nanostructured Metasurfaces

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ABSTRACT

We present a new class of materials in the form of ultrathin nanostructured metallo-dielectric metasurfaces that can manipulate the polarization state of light and produce giant rotation of polarization with relatively low loss. These subwavelength thick materials are formed from planar arrays of metamolecules that consist of achiral plasmonic nanostructures encapsulated within a chiral-patterned lossless dielectric layer. At plasmon resonance, the subwavelength nanoinclusions produce enhanced polarization of the surrounding dielectric, which gives rise to a rotation of polarization in the transmitted field. We use full-wave field theoy to demonstrate proof-of-principle for a prototype material that consists of a two-dimensional array of chiral Z-patterned metamolecules that contain a gold nanorod incluion. We also discuss applications of the metasurfaces to biosensing.

Keywords: metasurface, plasmonics, rotational of polarization, plasmon-enhanced linear birefringence, chiral metamaterials

1 INTRODUCTION

Advancements in nanotechnology have enabled the realization of unique artificial metamaterials with extraordinary optical properties such as negative refraction[1], slow light and cloaking[2,3] etc. Metamaterials hold promise for transformative advances in the fields of optical imaging, sensing, communications, computing and stealth technology, among others. In this presentation, a method is discussed for realizing ultra-thin (sub-wavelength) metasurfaces that can be tailored to control the polarization state of light and produce frequency selective giant polarization rotation with relatively low loss. The ability to control optical porlaization in this fashion opens up opportunities for the miniaturization of optical components such as wave plates, polarization rotators, and circular polarizers, thereby enabling new micro-optic applications that cannot be realized using conventional optically-thick components. To date, various metamaterials have been demonstrated that can be used to control optical polarization based on extraordinary linear or circular birefringence. Examples include metallic films with subwavelength apertures [4,5], metasurfaces with arrays of anisotropic metallic nanostructures and planar chiral metamaterials (PCMs) that consist of planar arrays of chiral metamolecules[6-10]. Many of these materials suffer from high loss, whereas the metasurcaes presented here provide comparable performance with relatively low loss due to a more limited use of metallic constituents. We use numerical full-wave field theory to demonstrate proof-of-principle of a prototype metasurface design and discuss biosensing applications of these materials.

2. METASURFACE DESIGN

A prototype metasurface design is shown in **Fig. 1**. This consists of a planar 2D array of chiral Z-shaped dielectric metamolecules on a loss-less dielectric substrate. Recall that an object is said to be chiral if it cannot be superimposed with its mirror image using rotations and translations alone. Helices, DNA molecules and the crystal lattice of quartz are examples of 3D-chiral structures. The Z-shapped metamolecule that we consider, absent the substrate, is not 3D chiral as it can be rotated out of the plane into their mirror image. Instead, it is chiral in a 2D or planar sense, since it cannot be superimposed with their mirror image using rotations or translations confined to the plane. However, the addition of the substrate breaks the out-of-plane rotational symmetry and renders the material 3D chiral. The Z metamolecules contain an embedded



Figure 1. Linearly polarized light (E₀) incident on a 2D array of dielectric chiral Z-structures with embedded gold nanorods producing elliptically polarized transmitted light with the rotation of polarization azimuth Δ .

achiral gold nanorod along their length. We study polarization rotation using numerical field analysis as illustrated in Fig. 1. Here, a linearly polarized plane wave with the electric field E_0 at an angle ϕ_{pol} with respect to the x-axis is incident on a metasurface. We show that this medium gives rise to an elliptically polarized transmitted field and we compute the rotation of the polarization azimuth in the transmitted field as the angle Δ between the semi-major axis of the ellipse and the incident polarization as shown. The Z metamolecule is a 2D extrinsic chiral structure that has C₂ rotational symmetry with respect to the direction of propagation, i.e. the z axis. It possesses linear birefringence, due to the anisotropic optical properties of the metamolecules, and circular birefringence because these 2D chiral structures reside on a substrate, which renders the media 3D chiral. These surfaces also possess frequency dependent linear dichroism due to the absorption properties of the embedded Au nanorods. We show that they can be tailored to exhibit giant polarization rotation due to plasmon-enhanced linear birefringence.

The computational model of a single Z metamolecule is presented in **Fig. 2**. Figure 2a shows surface plots of E_y and in the incident and trasmitted field. Figure 2b is a plot of the the induced polarization P_y that gives rise to E_y . We study a



Figure 2. Z metamolecule: (a) computational model and field analysis showing E_y in the incident and transmitted field for a unit cell with the incident polarization along the x-axis ($\phi_{pol} = 0^\circ$), (b) plasmon-enhanced polarization P_y , orthogonal to the incident polarization.

single dielectric Z metamolecule with the height of 200 nm, width of 300 nm, length of 350 nm along the x-direction and length of two short segments (s) of 180 nm along the ydirection. The dielectric is lossless and has an index of refraction of n = 1.6 to emulate the property of a conventional negative photoresist SU8. The embedded gold nanorod is 200 nm long and 80 nm wide and is located in the center of the long segment of the Z-structure as shown. The metamolecule resides on a lossless glass substrate with an index of refraction of n = 1.5. Perfectly matched layers (PMLs) are applied at the top and bottom of the computational domain to reduce backscatter from these boundaries. The height of the domain between the PMLs is 1500 nm along the z-axis and the direction of propagation (k) is downward, in the -z direction. The x and ydimensions of the unit cell in this case are 600 nm each and periodic boundary conditions are applied at x and y boundaries to account for the 2D array of identical structures. We assume that the incident field is a uniform downward-directed plane wave that is linearly polarized at normal incidence[11,12].

The optical response is predicted using full-wave timeharmonic field analysis. We solve for the E-field, which satisfies

$$\nabla \times \left(\mu_r^{-1} \nabla \times \mathbf{E}\right) - k_0^2 \left(\varepsilon_r - j \frac{\sigma}{\omega \varepsilon_0}\right) \mathbf{E} = 0, \tag{1}$$

, where μ_r and ε_r are the relative permeability and permittivity of the various constituent materials, respectively. For gold nanoparticles at optical frequencies, $\mu_r = 1$ and ε_r is modeled using an analytical expression that is based on the Drude-Lorentz model and matches the measured optical response of gold[13]. The COMSOL finite element-based RF solver (www.comsol.com) is used for the analysis.

We first compute the rotation spectra of the metasurface with the incident polarization at three different angles, $\phi_{pol} = 30^{\circ}$, 45° and 60° and the transmittance spectrum for $\phi_{pol} = 30^{\circ}$. As shown in **Fig. 3**, the maximum rotation is $\Delta = 38.84^{\circ}$ at $\lambda = 980$ nm when $\phi_{pol} = 30^{\circ}$, which corresponds to a giant specific polrization rotation of 1.942 x10⁵ deg/mm. The transmittance is 43.52% at this peak. As a point of



Figure 3. Z metamolecule: rotation spectra vs. polarization (ϕ_{pol}) and transmittance at $\phi_{pol}=30^{\circ}$.

comparison, the specific rotation of quartz is 13.3 deg/mm at $\lambda = 730.7$ nm. The rotation sensitivity with polarization



Figure 4. Z metamolecule: ellipticity for $\phi_{pol} = 30^{\circ}$.

indicates that the linear birefringence, resulting from the low C_2 rotational symmetry, is dominant. This level of rotation is comparable to that reported for media containing purely metallic chiral metamolecules[14], however higher transmittance can be realized with the proposed media because of the relatively lower metallic content. The ellipticity η of the transmitted field for ϕ_{pol} = 30° is plotted as a function of wavelength in Fig. 4, which shows that the polarization state of the transmitted field has been converted from linear to elliptical polarization.

We also investigate the dependence of rotation on the lattice spacing between metamolecules. The rotation spectra for $\phi_{pol} = 30^{\circ}$ is computed as a function of the lattice spacing for square unit cells, 500 nm, 550 nm and 600 nm on a side. The result is plotted in **Fig. 5** and shows that as the lattice spacing decreases the peak rotation increases and the spectrum blue shifts to shorter wavelengths. This is due to the near-field plasmonic coupling between the longitudinal resonances of nanorods, analogous to exciton coupling in H-aggregates of organic chromophores[15]. To verify this, we repeated the analysis with all of the dielectric material in the computational domain replaced by free-space, i.e.



Figure 5. Z metamolecule: rotation vs. size of the unit cell for $\phi_{nol}=30^{\circ}$

leaving only a 2D array of nanorods. We observed a similar blue shift in the absorption spectra as the lattice spacing decreased.

3. **BIOSENSING**

The metasurface can be adapted for use as a biosensor. In this application the gold inclusions are only partially embedded in the dielectric with their top surface exposed to the ambient environment as shown in **Fig. 6a**. In this case, the lower half of the nanorod is embedded and an equal upper half is exposed. The exposed surface of the nanorod is further functionalized to bind to a particular target analyte. The metasurface containing an array of such structures is submerged in an aqueous medium that contains the analyte. As the analyte binds to the nanorod it forms a coating as shown in **Fig. 6a**, which will have a different refractive index than the ambient medium. If the analyte has a higher index than the carrier fluid, the plasmon resonance of the coated nanorod will red-shift and produce a corresponding shift in the polarization rotation spectra as



Figure 6. Z metamolecule biosensor (a) unit cell of the modified Z metamolecule with a biolayer capped gold nanorod protruding from top surface, (b) polarization rotation spectra as a function of refractive index of the biolayer.

shown in **Fig. 6b**. The shift in the peak rotation can be detected and calibrated to determine the change in refractive index due to the biolayer, which in turn reflects the presence of the target analyte. Therefore by monitoring the wavelength of the peak rotation in the transmitted field of the sensor, the presence and level of bound analyte can be quantified. The device sensitivity can be defined using the formula

Sensor Sensitivity =
$$\frac{\Delta\lambda}{\Delta n} \left(\frac{nm}{RIU}\right)$$
 (2)

which is based on the ratio of the shift in the resonant wavelength to the change in the refractive index of the coating[16]. Using the formula and the data from **Fig. 6b**, the sensitivity of the Z-metamolecule metasurface biosensor is calculated as 133 nm/RIU and its sensitivity is plotted in **Fig.7**. This value is comparable to other optical biosensors,

such as 2D photonic crystals sensor with 30 RIU and planar ring resonators with 212 RIU.



Figure 7. Sensitivity with respect to the rotation spectra and resonance shift.

4. CONCLUSIONS

We have introduced a new class of metasurfaces for controlling optical polarization at normal incidence, which includes the ability to convert linera to elliptical polarization. These materials are formed from arrays of sub-wavelength chiral-patterned dielectric metamolecules that contain achiral plasmonic inclusions. Giant polarization rotation can be obtained near the plasmon resonance of the inclusions, which is due to enhanced polarization of the encapsulating dielectric. These metasurfaces open up opportunities for the development of versatile ultra-thin media that can manipulate optical polarization for novel micro-optical applications. We have demonstrated that the metasurfaces can also be engineered for use in optical biosensing applications.

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