Plasmonic Metasurfaces with Tailored Linear and Nonlinear Building Blocks

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Abstract

Plasmonic metasurface is an array of sub-wavelength plasmonic particle which is designed to obtain unusual performances by employing the localized surface plasmon (LSP). The dependency of the LSP on the geometry and the material of the plasmonic sub-wavelength particle have opened a wide range of applications for plasmonic metasurfaces. In the first chapter there is brief review of metamaterials and plasmonic metasurfaces. In the second chapter we present the concept of transmitarray concentrator implemented in optics. Planar concentric loop antennas are used as the elements for a $21 \times 21$ array to concentrate the incident plane wave at a desired distance. Finite difference time domain is used to obtain the performance of the periodic array of each element on the transmitarray and then free space dyadic greens function is employed to find the field distribution at each point, to show the focusing behavior of the metasurface. Third chapter investigates the concept of multi-layered tripod frequency selective surfaces in infrared. A full wave analysis based on finite difference time domain technique is applied to comprehensively characterize the structure and obtain the performance for both normal and oblique waves (for TE and TM polarizations). The layered tripod structure can be envisioned as a mean to realize cascaded LC circuit configurations achieving desired filter performance. A wide stop-band IR nano-filter which is almost independent of incident angle and polarization is demonstrated. Chapter 4 is concentrated on a functional metasurface building block which is multi-material loops. Plasmonic nano loops has been shown to be a capable candidate for creating building blocks of metasurfaces to manipulate the light in desired ways. Concentric loops can couple to each other strongly or weakly based on the relevant designs. The low-coupled multi-material loop metasurface can be employed as a frequency selective surface with number of separated bands. On the other hand one can take advantage of high coupling between the loops to achieve two different resonances; one will be a high quality factor and sensitive mode and the other a radiating wideband low-loss resonance. In both resonances the building block has a sub-wavelength size. Here the performance of periodic array of multi-material loops is investigated by means of finite-difference time-domain technique. Based on the performance of a single plasmonic loop with general Drude material the behavior of the multi-material loop metasurface is investigated. We show how choosing the proper materials can control the resonance characteristics. The performance of multi-material loops is studied by
utilizing the induced net dipole moments on the concentric loops and appearance of Fano-like resonance in the high-coupled case is demonstrated. Moreover, the large field enhancement as a result of a subradiant resonance is studied. The sensitivity of the structure to the spacer layer permittivity and loss are investigated in details. And last but not least, the effects of breaking the symmetry in the multi-material loop building block are also examined. Excitation of the quadrupolar mode of the loop, Fano-like resonance and high intensity localized field are elucidated for the non-concentric multi-material loop building blocks. In chapter 5, the performance of multi-material loop metasurface integrated with Kerr nonlinear material is investigated comprehensively with finite difference time domain method. Optical bistability is obtained by exciting the metasurface with a saw-tooth profile for its amplitude. The effects of coupling between the plasmonic loops on the bistability curve are studied and the trade-off between the required intensity for switching and the extinction ratio of the two states of the switch is explored systematically. The dissertation is finished by a number of recommendations for the future directions for this research.
Dedication

I would like to dedicate this dissertation to the most beloved people in my life; my father, Javad, who showed me determination and hard work are the most crucial assets for success; my mother, Shahla, who taught me to love unconditionally; my sisters Bahar and Laleh, whom even when we were continents apart, I always felt their presence beside me with their immense support; and last but not least my lovely fiancé, Soudeh, who stood strong beside me during the toughest times of this journey.
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Chapter 1

Introduction

Plasmonic metasurfaces

The concept of metamaterials started when Veselago studied the behavior of wave propagation inside a material with negative permittivity and negative permeability in 1968 [1]. He showed that the simultaneous negative permittivity and permeability result in negative refractive index. From Maxwell’s equations it is easy to demonstrate that the vectors of $\mathbf{E}$, $\mathbf{H}$, and $\mathbf{k}$ in a negative index material form a left-handed triple which is the root of calling the negative refractive index materials as Left Handed materials [2]. Three decades later almost at the same time David Smith and his team at university of California in San Diego and John Pendry at Imperial College in London demonstrated the first fabricated structure that had negative effective dielectric permittivity and magnetic permeability [3, 4]. Resonating wires causes the negative permittivity and the negative permeability is achieved by employing split ring resonators. One of the well-known applications of left handed materials is super lensing which is accomplished because of the anti-parallel directions of Poynting vector and propagation vector [5]. Although the starting point of metamaterials was investigation of wave and matter interaction with negative refractive index, the definition of metamaterial is broader than this. By definition, any artificial material which has characteristics that cannot be found in nature is called metamaterial [2]. This broad definition has opened a huge gate for researchers to expand the science of artificial materials with the goal of achieving unusual characteristics.

Plasmonic metasurfaces, as one of the research areas in metamaterials, have attracted lots of attention among researchers. The conductive electrons of a metal at the interface of the metal with a dielectric can be excited by an incident electric field, which is classified as surface plasmon [6-8]. The excitation of surface plasmon can be employed in two different scenarios; one is wave propagation along the interface of the metal and
the insulator, surface plasmon polariton (SPP), which leads to the design of photonic devices and integrated optics. The other is localization of surface plasmon around a sub-wavelength plasmonic particle, localized surface plasmon (LSP), which is a resonance phenomenon [7, 8]. One of the remarkable examples of this field of research is the “metatronics” concept, the work of Engheta at university of Pennsylvania, which employs the surface plasmon to realize the lumped element circuits in optics [9, 10]. The localized surface plasmon (LSP) is mostly used in plasmonic metasurfaces where the resonance characteristics of the sub-wavelength particles are engineered to achieve features that are not realizable by materials in nature. For example, extraordinary performances such as optical cloaking, improving the efficiency of photovoltaic systems, wave steering, high resolution imaging, controlling the amplitude and phase of transmitted light have been obtained by just an array of plasmonic scatterers, which is known as metasurface in the community [11-16]. One of the main reasons of huge attention to metasurfaces is the challenge in fabricating the metamaterials. For metamaterials the effective constitutive parameters are obtained for a bulk materials. In other words, in order to obtain the effective permittivity and permeability the structure should have a thickness of several wavelengths in the propagation direction. This makes the fabrication of metamaterials challenging specially in terahertz and optical frequencies. However, the plasmonic metasurface fabrication does not face these challenges. The oscillation of the conductive electrons is demonstrated with the Drude model in the electric permittivity of the metal [17]. The materials that are being used in plasmonics are mostly noble metals; e.g. silver and gold. The loss of some noble metals near the optical communication window is significant. Also the real part of the permittivity of these materials is large in the near infrared (NIR) spectrum, which limits the use of them in this spectrum. Boltasseva and her group have discovered a new type of material, transparent conducting oxides, e.g. indium tin oxide (ITO) to overcome the issues of loss and the large permittivity in noble metals in NIR [18].

Finite difference time domain (FDTD) technique is a powerful tool in investigating the performance of different metasurfaces for a number of reasons. The ability of modeling dispersive materials with auxiliary differential equations (ADE) method have made it possible to model the permittivity and permeability of different materials with
multi-pole Drude-Lorentz function that can be fitted to data available in the literature. The time domain nature of this technique would save a lot of time in obtaining the performance of a metasurface in the desired range of spectrum with just one simulation. Furthermore, the Yee’s algorithm can be modified in order to simulate the third order nonlinearity and obtaining the bistability curve. Therefore, the home-developed three-dimensional FDTD code that is capable of modeling dispersive and nonlinear material is used for most of the investigations in this dissertation. The code is implemented on a graphical processing unit (GPU) to boost up the speed significantly [19, 20].

**Planar optical lenses**

Focusing the light beyond the diffraction limit is highly desired in many applications such as high-resolution imaging and photovoltaic [13, 21, 22]. Traditionally the light was focused by means of the curved dielectric lenses. With this method the light can be focused on a spot greater than half of the impinging light wavelength due to the diffraction limit [23]. The curvature of the lens compensates the phase of the impinging plane-wave so that the phase-front on the other side of the lens forms a circular pattern. Beside the diffracted limited focal point, the fabrication challenges and the compatibility for integrated optics application make the planar lenses more desired compared to the conventional curved ones [24]. On a plasmonic metasurface the desired-phase front can be achieved by engineering the sub-wavelength plasmonic inclusions. In other words, on different locations of the array, a proper inclusion is implemented to compensate the phase due to different path lengths to the focal point. In the second chapter of this dissertation, a transmitarray metasurface is design with the goal of focusing the light. For the sub-wavelength inclusions, concentric rectangular loops are considered because of the large achievable phase change by engineering the dimensions of the rectangular loops. The performance of the periodic array of the building block as a function of different parameters (dimensions) is obtained by means of FDTD. Due to the large dimension of the designed array, the field distribution of the transmitted light is calculated by use of the Equivalence theorem and free space Green’s function.
Plasmonic frequency selective surfaces

Microwave frequency selective surface (FSS) is known as the root of metamaterial tree of knowledge [25]. The FSS is a periodic array of scatterers that filter specific frequencies. Combining the FSS concept with the well-known filter theory has enabled possibility of cascading different layers of FSS to achieve wideband characteristics [26]. On the other hand, highly reflective mirrors with wideband characteristics are greatly desired in applications such as sensors, imaging, telecommunications, and surveillance [27, 28]. In the third chapter of this dissertation, the enriched concept of FSS in microwave complemented by filter theory are combined with plasmonics to design an ultra-wideband nano-filter to reflect the impinging light with more than 80% reflectivity. Owing to the symmetric shape of the tripod, the building block of this metasurface, the performance of the filter is independent of incident angle and light polarization. A circuit model is proposed based on the physics obtained by near field distribution that can help to better understand the governing physics and possibly the ways to optimize the designed filter.

Multi-material loop metasurface

Dependence of the LSP resonance to both geometry and material of the plasmonic subwavelength particle makes these two parameters as the principle features that can be engineered to achieve the anticipated design [29]. One can also take advantage of the near field enhancement at the interface of the plasmonic and dielectric materials by perturbing the coupling between the adjacent plasmonic particles [30-32]. The coupling between these inclusions can be predicted by means of hybridization model proposed by Nordlander et. al. in [33]. The fourth chapter of this dissertation is the report of a comprehensive study on the multi-material loop metasurface. The building block of this metasurface is a number of concentric plasmonic loops with spacer layers in between them. Parameters such as the aspect ratio and the material of each loop offer a large degree of freedom in design. Although at the first glance the fabrication looks very challenging, the work by George Whitesides group made us more confident about the feasibility of this design [34]. Based on the coupling between the plasmonic loops we divide this study into two categories; low coupled and high coupled designs. In the low-
coupled design, each resonance is controlled individually by perturbing the corresponding resonating loop. Different materials can be used for the plasmonic loops to change the resonant spectrum with respect to the materials plasma frequency. On the other hand, in the high-coupled design, each resonant frequency does not correspond to one resonating element as the loops are are highly coupled to each other. As a result it is possible to have a very narrow-band resonance within a broadband one to obtain a Fano like resonance. The net dipole moment induced on the surface of the building block is very informative in regards of field enhancement, bandwidth, and sensitivity of the resonance. In the high-coupled design, the resonances have completely different features; a subradiant resonance that has a narrow bandwidth and huge quality factor and a superradiant resonance with wide bandwidth and low loss. Each of these resonant features can be employed in different applications such as sensing, nonlinear optics and photovoltaic systems. Effects of perturbing the space layer permittivity and adding loss to the space layer are studied for both designs. Moreover, the effects of breaking the symmetry in the multi-material loop building block are investigated.

**Optical bistability in multi-material loops**

Optical nonlinearity is the foundation for optical signal processing, all optical switching and quantum mechanics [25, 35, 36]. In general form the polarization vector or the dipole moment per volume of a material depends on the strength of electric field. Equation (1.1) describes this nonlinear dependence [36].

\[
\vec{P}(t) = \chi^{(1)} \vec{E}(t) + \chi^{(2)} \vec{E}^2(t) + \chi^{(3)} \vec{E}^3(t) + ... = \vec{P}^{(1)}(t) + \vec{P}^{(2)}(t) + \vec{P}^{(3)}(t) + ...
\]  

(1.1)

where \(\vec{P}^{(1)}(t)\) is the linear polarization term and \(\chi^{(1)}\) is the linear susceptibility, \(\vec{P}^{(2)}(t)\) and \(\vec{P}^{(3)}(t)\) are the second and third order nonlinear polarization vectors, respectively. Moreover, \(\chi^{(2)}\) and \(\chi^{(3)}\) are the second and third order nonlinear susceptibilities, respectively. It is noteworthy that in equation (1.1) the susceptibilities are assumed to be independent of time. That means the polarization vector depends only on the immediate strength of the electric field. This assumption will lead to considering the material as a lossless and non-dispersive material. Generally the values of the second,
third and higher order susceptibilities are very small due to their principle mechanism of photon-photon interaction. The materials with inversion symmetry such as liquids, gases, and amorphous solids do not have any second order nonlinear interaction with light, as their second order susceptibility is zero. The second order nonlinearity will result in second harmonic generation, sum and difference frequency generation, electro-optic effect, etc. The results of third order nonlinearity are four wave mixing, third harmonic generation, and Kerr effect which is a perturbation in the permittivity of the material by the applied electric field intensity. The later effect is mainly used in designing all optical switches and modulators. Combining the Kerr effect with a feedback mechanism results in two steady states for the same input intensity, which is called optical bistability [35, 37-40]. Due to the very small value of the nonlinear susceptibilities, these effects would come to the picture only when the intensity of the electric field is large enough [35, 36]. Therefore, plasmonic metasurfaces are one of the great candidates for optical nonlinearities due to enhancement of localized electric field. In chapter 4, we show the capability of the multi-material loops building block in enhancing the localized electric field when the coupling between the plasmonic loops is large. It is also elucidated that for the high-coupled design, changing the refractive index of the spacer layer would result in a redshift in the first resonant frequency while the second resonance remains unchanged. In the fifth chapter of this dissertation, the multi-material loop building block is integrated with Kerr nonlinear material to obtain optical bistability. The more the coupling between the plasmonic loops, the higher field enhancement is achieved within the spacer layer. However, that does not guarantee a better performance in the switch. Through our study we show that by increasing the coupling in multi-material loop building block, although the required input intensity for switching decreases, the extinction ratio of the optical switch is diminished as well.
Chapter 2

Concentric rectangular loops for light focusing

**Introduction**

Light concentration is the key for a variety of applications such as solar cells [13], high-resolution imaging, and optical sensors [41]. Previously, in order to focus the light, dielectric shaped lenses were used. Because of the diffraction, the focal area of the dielectric lens is more than half of a wavelength, which results in lower light intensity [21]. A transmitarray is a planar substitute for dielectric shaped lenses to collimate and focus an incident light beam. The planar shape of the array makes it easier for manufacturing and integration with other parts of the system compared to the traditional dielectric shaped lenses [42]. Looking at a transmitarray as a device to give directive beam in a specific direction, the phase of the elements should be such that the phase delays corresponding to the different path lengths can be compensated and a constant phase on the array aperture is established. By reciprocity, light concentration can be achieved, illuminating the array with a plane wave.

In optics, there have been several attempts to achieve focusing with the use of thick plasmonic structures, e.g., slit arrays [42-45], an array of holes with different shapes in metallic films [46-48], and metallic pillar arrays [49]. In these works, they use guided waves through metallic films or pillars to obtain the required phase change. In this Letter, we introduce a novel planar configuration, which is more desirable and easier for fabrication, based on the concept of transmitarray enabled in optics. There are significant works in microwave to realize such an array by different elements like stub-loaded patches, crossed dipoles, and double-ring resonators [50]. In the near-IR and optical regimes, the metal cannot be treated as a perfect electric conductor. According to Drude model, the electric permittivity of metal has a negative real part in the wavelength of interest. This phenomenon can be used to excite the surface plasmon polaritons for the scatterers in the array. To tailor the required phases on the aperture, different elements
with different transmission phase delays should be placed at desired array locations. The amount of the required phase delay on the whole aperture depends on the dimensions of the array and the distance of the focal point to the array. Finding a unique scatterer with the ability of changing the transmission phase by perturbing its shape (changing the dimensions) in the near-IR is an important task that is addressed here. In this chapter, a design for a polarization-independent transmitarray antenna with means of planar concentric loop antennas (depicted in Figure 0.1) is investigated numerically. A three-dimensional finite-difference time-domain (FDTD) technique with periodic boundary condition is used to obtain the transmission amplitude and phase of different configurations for the unit cell designs in a periodic fashion [19, 20]. The unit cell size is 200 nm with the substrate thickness of 150 nm. To obtain the maximum phase change over the aperture, the concentric rings are placed on both sides of the substrate. Then, a non-uniform array of $21 \times 21$ elements is designed, and the focusing performance at $2\lambda$ away from the structure is illustrated. This array is designed to operate at 1.55µm wavelength.

![Diagram](image)

Figure 0.1: Schematic of the unit cell (of a periodic structure). (a) yz plane and (b) xz plane.
Unit cell design and simulations

The required phase change on the transmitarray located in the yz plane and illuminated by a plane wave propagating in the x direction can be calculated by equation (2.1), where the y and z are the coordinate of the center of the element in the array and f is the focal distance from the center of the array. Besides the required phase delay that is needed for focusing, the amplitude of the transmitted wave should be close to 1. That means the unit cell design should have 0 dB transmission with the required phase according to its position on the array

\[ \phi(y, z) = \frac{2\pi \sqrt{f^2 + y^2 + z^2}}{\lambda} - \frac{2\pi f}{\lambda} \]  \hspace{1cm} (2.1)

Recently, Ahmadi and Mosallaei have shown the performance of a single and array of loop antennas in optics [51]. Obviously the resonant frequency of the loop antenna depends on the arm length of the loop, the thickness, and also the width of the arms [29]. This dependence makes the loop antenna an ideal element for the array design because the idea is to change the resonant frequency for different elements by engineering its parameters. Hence, the transmission phase will change at the working wavelength, which is 1.55µm. By introducing another loop inside the first one, a second resonant frequency will come up in the transmission spectrum. The effect of the second resonant is to increase the slope of the transmission phase versus frequency between two resonances and increase the design flexibility. In this case, the higher phase change can be gained by tailoring the loops parameters. Figure 0.1 shows the schematic of the unit cell (of a periodic structure) and the parameters that can be changed to obtain the phase delay. A higher amount of phase change is determined by printing two concentric loops layers on both sides of the substrate [see Figure 0.1(b)]. This leads to higher bandwidth resonance and also higher slope of the transmission phase versus frequency.

The FDTD method is applied to model the unit cell. The computational domain is configured with cubic Yee cells with the dimension of \( \Delta = 2.5 \) nm. The unit cell is assumed to be periodic in the y and z directions. A plane wave having a z-polarized electric field is illuminating the unit cell in \(-x\) direction. The fields are read at 10 cells
away from the slab on the other side, and the transmission amplitude and phase are evaluated. The substrate is made of dielectric with low permittivity of 1.4 [52], and the loop elements are made of Silver. Silver is modeled with Drude material with plasma frequency of $\omega_p = 2\pi \times 2175\text{THz}$, damping factor of $\gamma_p = 2\pi \times 4.35\text{THz}$, and $\varepsilon_\infty = 5.0$ [53, 54]. There are four parameters to be optimized to achieve the required phase values at proper locations within the array. To make the study easier, two of them are optimized and fixed, which are the width of the inner and outer loops, $T_i = 5\text{nm}$ and $T_o = 20\text{nm}$. In Figure 0.2 the transmission amplitude and phase versus frequency is illustrated for two different configurations that are $L_o = 150 \text{nm}$, $L_i = 50 \text{nm}$ and $L_o = 150 \text{nm}$, $L_i = 25 \text{nm}$. The key is to have around 0 dB transmission magnitude, which is satisfied at 193 THz. By decreasing the inner loop arm length, the second resonant shifted toward lower frequencies, and hence there is a phase change in the transmission phase at 193 THz for these two different configurations.

![Figure 0.2: Transmission (a) amplitude and (b) phase versus frequency. The blue solid curve is for $L_o = 150 \text{nm}$ and $L_i = 25 \text{nm}$. The red dashed line is for $L_o = 150 \text{nm}$ and $L_i = 50 \text{nm}$.](image)

Two unique designs are studied here; fixed outer loop arm length ($L_o$) while changing the inner loop arm length and vice versa. In the first design, the outer loop arm length is fixed at 150nm, and the inner loop arm length is changed from 25nm to 55nm. In the other one, the inner loop arm length is fixed at 35nm and the outer loop arm length is varied from 100nm to 125nm. For each configuration, the transmission amplitude and
phase are obtained by means of FDTD. Note that, due to the FDTD meshing, the changes in the arm length are discrete. Hence, after finding the transmission amplitude and phase for the possible configurations in FDTD, for other values of arm lengths, the piecewise cubic Hermite interpolating polynomial function embedded in MATLAB is used. In Figure 0.3, the obtained results by FDTD are shown by markers on top of the curve which is the outcome of the interpolation.

Figure 0.3: Study of changing the parameters of the unit cell to obtain required transmission phase. (a) The transmission amplitude and (b) phase for the first design ($L_o = 150\text{nm}$, $25\text{nm} < L_i < 55\text{nm}$). (c) The transmission amplitude and (b) phase for the second design ($L_i = 35\text{nm}$, $100\text{nm} < L_i < 125\text{nm}$).

As can be seen from Figure 0.3, a transmission phase change of about $160^\circ$ can be achieved. However, by looking at the transmission amplitude, it is obvious that we are limited to the cases that have transmission amplitudes at least greater than $-6 \text{ dB}$ (to achieve better focusing). Note that, by moving toward the corners of the array, the
transmission amplitude could be tapered in order to avoid diffraction from the edge of the slab. Hence, the -6 dB transmission amplitude is acceptable if the corresponding element is placed far from the center of the array.

**Transmitarray metasurface design**

Having the data for each unit cell, an array of $21 \times 21$ elements is designed to concentrate the light at a distance of interest. At the center of the array, an element with the highest transmission amplitude should be placed. For the phase, the center element phase delay is the base, and the other phase delays are considered with respect to the center one. Using equation (2.1) and the obtained FDTD phase results, suitable design for the elements of the array is found. A schematic of the array of $21 \times 21$ elements and the phase performance approximated by the data obtained by unit cell simulations are illustrated in Figure 0.4. For the elements at the center of the array, the magnitude should be as close to 0 dB as possible. Also, the fact that the required phase delay is increasing by moving toward the corners of the array tells us the center element should have the highest negative phase delay. These two reasons lead us to use the first design (fixed outer loop) for the elements at and near the center of the array. By going toward the corners, the second design (fixed inner loop) is used.
Figure 0.4: (a) Schematic of the 21 × 21 array elements for focusing the light. Note that the scatterers are placed on both sides of the substrate. (b) The required phase delay and (c) the obtained phase delay by the array of scatterers.

It must be mentioned that, although here a non-periodic array is designed, each element can locally be considered as periodic and the obtained simulation for the amplitude and phase of the periodic structure can successfully be used. This approach is known and has been validated extensively in literature [11, 49, 50, 55, 56]. Let us now calculate the field intensity of the array structure. Because of the large size of the array, it is not efficient to model the structure using the FDTD method. Instead, we apply the field equivalence principle [57] to obtain the tangential fields on a surface close to the array, and from that the field performance at any place in space is obtained, efficiently and accurately. To achieve this, the electric and magnetic current densities J and M from the
periodic modeling are used on the aperture of the finite array structure, and by using proper dyadic Green’s functions, the field at any place is determined:

\[
E = \int G_e^1 \cdot \vec{J} dr + \int G_{em}^1 \cdot \vec{E} dr
\]  

(2.2)

The light concentration of the transmitarray configuration is shown in Figure 0.5. The focusing is at 2\( \lambda \) away from the slab. Focal distance can be engineered by tailoring the dimension of the array. Increasing the number of elements and using more layers can generate larger phase variation, enabling focusing with better resolution and at desired distance. It should be mentioned that the fabrication of our proposed concentrator is more convenient than other available alternatives. This is mainly because of the planar configuration of the structure and being free of needing large aspect ratio plasmonic elements.

**Conclusion**

In this chapter, the concept of transmitarray antenna enabling light concentration in the near-IR region is explored. As for the elements of the transmitarray, concentric rectangular loop scatterers are chosen due to their design flexibility and potential for providing high phase variation by changing the dimensions of the loops. Periodic behaviors of the concentric loop elements are obtained by means of the finite-difference time-domain method. Using these results, a transmitarray configuration is designed, and a focused beam at a desired distance is achieved. To model the electromagnetic fields of finite array, field equivalence principle and proper dyadic Green’s functions are applied.
Figure 0.5: Electric field distribution after the concentrator in (a) xy plane, (b) xz plane, and (c) yz plane (at the focal plane).
Chapter 3

An ultra-wideband filter comprising plasmonic tripod metasurfaces

Introduction

Light manipulation using surface plasmon polariton (SPP) is of great interest in IR-Optics featuring novel applications. By patterning a layer of plasmonic material in an appropriate way one can employ the SPP in order to reflect or transmit the electromagnetic waves over specific bands of frequencies. The concept of frequency selective surfaces (FSSs) is of great benefit to enable this importance [25, 26]. Looking at variety of FSS applications in infrared (IR) spectrum; e.g. solar cells [13], high resolution color filtering and spectral imaging [58], optical sensors [59], high directive terahertz antenna [60], earth observation remote sensing instruments [61], and energy saving glasses [62], will give scientists the motivation to design novel FSSs for specific purposes; for instance broadband performance which is independent of the excitation’s polarization and angle of incidence. The filter like behavior of the FSS will bring up the possibility of making sophisticated designs utilizing the concept of filter theory in circuits. Basically, by combining different resonant elements in novel fashions one would be able to achieve broadband characteristics. We will utilize this concept to achieve plasmonic patterns acting like nano-filters in IR. In order to better understand the physics behind each design, we will propose a circuit model which we can clarify the performance of the design by that.

Considering the complexity of the FSS structures and the fact that they are made from plasmonic materials with dispersive characteristics one would need to apply a powerful computational technique to solve the problem accurately and efficiently. Here, a Finite Difference Time Domain (FDTD) technique is applied [19, 20]. One of the excellent advantages of FDTD for FSS characterization is that it is a broadband analysis. This means obtaining the whole frequency response of the filter with one simulation run.
By using auxiliary differential equation (ADE) method, we model the plasmonic material with Drude function of \( \varepsilon(\omega) = \varepsilon_{\infty} - \omega_p^2 / (\omega^2 - j\gamma_p \omega) \). In our study, we consider Silver with plasma frequency of \( \omega_p = 2\pi \times 2175 \text{THz} \), damping factor of \( \gamma_p = 2\pi \times 4.35 \text{THz} \), and \( \varepsilon_{\infty} = 5.0 \text{ THz} \) [54]. The periodic boundary condition (PBC) and convolutional perfectly matched layer (CPML) absorbing walls are used to terminate the computational domain. The absorption of the CPML has been shown to be almost independent of the media even if the media is inhomogeneous, lossy, dispersive, anisotropic, or nonlinear [19]. By considering 20nm for the FDTD cell size the effect of staircase meshing becomes negligible in modeling the triangle edges of the designed structures. The incident source is implemented by total field scattered field (TFSF) technique [20]. This technique allows us to separate the incident field from the total field in the reflection side and hence with one simulation we can obtain the reflectivity which is the backward scattered field. In order to simulate the oblique incidence, we have used the Sine-Cosine method to overcome the causality problem in the formulations [20, 63]. However with each simulation with Sine-Cosine method, the obtained results are for one specific frequency. Therefore the sweep in the desired frequency range is needed.

We study the performance of an FSS build from a single layer of plasmonic tripod. Based on the field distribution we compare the performance of the FSS with a series LC circuit. By adding another layer we design a metasurface building block which can resemble two coupled resonances of two series and parallel LC circuits. The effect of strong coupling between the two layers is studied. Cascading two or more blocks of this metasurface properly would give us the ability to engineer the performance over the frequency range of interest. An almost polarization independent and wide-angle nano-filter with a broad stop-band and sharp rising and falling edges is achieved. We investigate the effect of oblique incidence for both polarizations, namely TE (Electric field polarized along z direction) and TM (Magnetic field polarized along z direction) and explain the behavior of the nano-filter for these different cases by exploring the field distributions.
Single and double layer of plasmonic tripod metasurfaces

An FSS made of an array of plasmonic tripods in hexagonal lattice is shown in Figure 0.1(a). This array is embedded in a lossy dielectric medium with relative permittivity of $\varepsilon_r = 1.96 + j0.1$ and thickness of 700nm. The arm length of each tripod is assumed to be 480nm and the arm width is considered 400nm. The unit cell size in y and z directions is 1.40µm and 2.44µm, respectively. The unit cell of the periodic array (Figure 0.1(b)) is illuminated by a plane wave propagating in −x direction with electric field polarized along z direction (TE polarization). The FDTD is applied and reflectivity ($|E_{\text{Ref.}}/E_{\text{Inc.}}|^2$) is obtained in Figure 0.1(c). The peak is at the point where the plasmonic tripod goes to resonance. The behavior of the tripod FSS could be better understood with its circuit model. A single layer of the array of tripods can be considered as series LC circuit configuration, as shown in the inset of Figure 0.1(c). The current flow on the tripod leg provides L and the electric field coupling between the elements offers the required C for resonance [64]. The calculated S-parameter from this circuit model is shown as dashed lines in the Figure 0.1(c). A relatively good comparison is illustrated. The difference in the amplitude is due to the loss which is considered in full wave analysis but not for the circuit model (for the sake of simplicity of circuit representation). The near field results for E and H on tripod are shown in Figure 0.1(d) and (e). Strong electric field at the tripod gaps and magnetic field on the tripod legs are shown.
Figure 0.1: (a) The schematic of the proposed tripod FSS. (b) The unit cell of the periodic array. The dashed lines are representing the periodic boundary conditions in y and z directions. The unit cell sizes in y and z directions are $T_y = 1.4$ $\mu$m and $T_z = 2.44$ $\mu$m, respectively. The arm length and width are assumed to be $L_1 = 480$ nm and $L_2 = 400$ nm as defined in the figure. (c) The solid line is the reflectivity of the plasmonic tripod FSS obtained with FDTD. The dashed line shows $|S_{11}|^2$ calculated for the shown series LC circuit with $C = 0.0039$ fF and $L = 667$ nH. The tangential (d) electric and (e) magnetic field at resonance on the surface of the periodic array unit cell show the coupling between the legs of the tripods and the current flowing on the tripod legs, respectively.

By introducing another layer of plasmonic tripod very close to the first layer with 180 degree rotation with respect to the x axis and a shift in z direction in a way that each arm in the first layer would have overlap with one arm in the second layer, there would be a strong coupling between these two plasmonic layers. This coupling could be engineered by changing the distance between the two layers or changing the overlapping area of the tripod legs. Having the second layer rotated gives us more flexibility to control the overlapping area between the tripod legs of the two arrays [65]. The two layer structure and the unit cell are shown in Figure 0.2(a) and (b), respectively. The reflectivity illustrated in Figure 0.2(c), shows an enhancement in the bandwidth and a shift-down in the resonant frequency. The shift in the resonant frequency of the double
layer design and also the increment in the bandwidth are all the result of the strong introduced coupling between the two layers. To show these effects in the circuit model, we propose two LC resonators as depicted in the inset of Figure 0.2(c). The series LC shows the behavior of the plasmonic tripod metasurface while the shunt LC represents the effect of the coupling between the two layers (due to strong electric field between them). The calculated S-parameter of the circuit is illustrated by dashed line in Figure 0.2(c). Note that in this configuration the capacitances (C1 and C2) are coupled due to the strong coupling between the two layers. Therefore, the values used in the circuit models for one layer and two layers are different. The ripple observed in the calculated S-parameter can be attributed to the considering no loss in the circuit model, as loss can always couple the poles in a better form (removing the zero between the resonances). The tangential fields are shown in Figure 0.2(d) and (e). Strong electric and magnetic field intensities are observed. Also note that for the two layers case the current can be conducted from the tripod in first layer to that in second layer through the C coupling between them (and as such a stronger magnetic field on the legs of tripod in compared to the one layer case is observed). It must be mentioned that one might be able to obtain a more complex circuit configuration to very accurately duplicate the FDTD performance of the two layers tripods, but in this work our goal has been to provide a simple and yet proper representation of the system including the main physics of structure.
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Figure 0.2: (a) The schematic of the two layer plasmonic tripod FSS embedded inside the dielectric. (b) The unit cell of the periodic array. (c) The solid curve is the reflectivity for d = 40nm obtained by FDTD. The dashed line shows the $|S_{11}|^2$ calculated for the circuit with $C_1 = 0.0041 \text{ fF}$, $L_1 = 1.3 \text{pH}$, $C_2 = 0.0038 \text{ fF}$, and $L_2 = 3.8 \text{pH}$. The tangential (d) electric and (e) magnetic field at resonance on the surface of the periodic array unit cell shows high field intensity at some new spots which represents the coupling between the two layers.

Increasing the distance between the two layers, results in decreasing the coupling between them. Based on the circuit model, the capacitances of the circuit are decreasing which results in shifting up in the frequency. In order to validate this phenomenon we have obtained the reflectivity for three different values of d (the distance between two layers) as shown in Figure 0.3(a). As we expected, the results show us the shifting toward higher frequency in the resonance of the FSS. The x-component of the electric field between the two layers of the tripod is enhanced significantly. This fact is shown in Figure 0.3(b) where the electric field in x direction is shown between the two overlapped legs of the two layers in xz plane. The yellow dashed lines showing the boundaries of the tripod leg in both arrays. Note that here the amplitude of the electric field in x direction is 5 V/m although the incident electric field is polarized along z direction (TE). This clearly shows the strong coupling between the two layers and also another proof of the capacitance C2 proposed in the circuit model. This two layer tripod is a metasurface.
building block acting as an FSS with two coupled resonances according to its proposed circuit model. Note that the thickness of the building block is far less than the resonant wavelength in free space (0.02\(\lambda\)). This would give us the possibility of cascading couple of these metasurface building blocks in order to achieve a flat stop band filter behavior, while the thickness of the structure is still very small compared to the center wavelength.

![Figure 0.3](image)

**Figure 0.3:** (a) The reflectivity for three different values of \(d\) showing the effect of decreasing the coupling between the two layers by increasing the distance between them. (b) The \(x\)-component of electric field in \(xz\) plane between the two overlapped legs of tripod in each layer. The yellow dashed lines are the boundaries of the tripod legs. The enhanced electric field counts as a result of the coupling between the two adjacent layers.

**IR Nano-Filter**

According to the filter theory, by cascading multiple resonators, one can engineer a broadband filter with a flat pass/stop band behavior [26, 66]. This needs special design such that the poles of the resonant elements are coupled in a proper way. To achieve this we cascade two of such layers in a distance \(D\) from each other, as depicted in Figure 0.4(a). In Figure 0.4(b) we show the effect of \(D\) by obtaining the reflectivity for different \(Ds\) while \(d\) is fixed (\(d = 60\)nm). Increasing the \(D\) will decrease the upper edge frequency. In Figure 0.4(c) the effect of \(d\) is investigated for a fixed \(D\) (\(D = 900\)nm). Increasing the \(d\) will increase the lower edge frequency. For the rest of the study based on the aforementioned observations we have chosen the parameters \(d(40\)nm\) and \(D (700\)nm\) in order to have a nano-filter with larger than 80% reflecting the impinging light intensity from 30 THz to 85 THz. It has also sharp rising and falling edges.
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First we cascade two of the circuit model proposed for two layers tripod design with a 700nm long transmission line as illustrated in Figure 0.5(a). The agreement between the reflectivity of the nano-filter and the performance of the circuit is shown in Figure 0.5(b). Here because no loss for the circuit model is assumed the stop band performance is very flat. In presence of loss the edges of the stop band is not as sharp as what the circuit model obtains and also the amplitude of the S11 is decreased. These effects can be seen in the FDTD results where we have taken the loss of the Silver and also the dielectric into account. We need to also mention that increasing the length of the transmission line has the same effect as increasing the D in the actual design. Overall a good comparison between the actual configuration and circuit model is observed (the circuit model cannot take into account all the electromagnetic details and edge diffractions of course). The symmetric shape of the layered tripod results in the independency of the nano-filter to the polarization state. In order to show this we obtain the performance of the proposed design for the other polarization which has the magnetic field along z direction (TM polarization). As shown in Figure 0.5(b) the reflectivity for the both polarizations are almost the same.

Figure 0.4: (a) The schematic of the four layer plasmonic tripod nano-filter. (b) Reflectivity for three different values of D while d is assumed to be 60nm. (c) Reflectivity for three different values of d while D is assumed to be 900nm.
Figure 0.5: (a) Circuit model for the designed nano-filter. The transmission line has a length of 700nm with the characteristic impedance of 269.3ohm. (b) The solid curve corresponds to TE polarization and the dashed curve is for TM. The dotted line is the calculated $|S_{11}|^2$ of the circuit model with the parameters of $C_1 = 0.0041 \text{ fF}$, $L_1 = 1.3 \text{ pH}$, $C_2 = 0.0038 \text{ fF}$, and $L_2 = 3.8 \text{ pH}$.

The response of the nano-filter to oblique wave is also explored. We change the azimuthal angle ($\phi$) from 10 to 60 degree for both polarizations (TE and TM). As shown in Figure 0.6, the TE polarization is less sensitive to the angle of incidence compared to TM polarization. For the TE polarization the electric field remains along z direction and by increasing the azimuthal angle the x-component of the magnetic field will increase. However, for the TM polarization increasing the azimuthal angle results in increasing the x-component of the electric field (the normal component to the surface) and the magnetic field is along z. Since the normal component of electric field is associated with charge accumulation on the surface (in contrast to the tangential E or normal H) one would expect dependency on angle of incidence to be more dominant for the TM polarization than the TE. The results in Figure 0.6 clearly illustrate this. Nevertheless up to 60 degree a relatively wideband stop-band performance is obtained. The similar phenomenon should be observed for changing the angle in other plane due to the symmetricity in geometry.
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Figure 0.6: (a) TE and (b) TM reflectivity from the nano-filter excited with oblique incident planewave.

Conclusion

In this chapter we present the design of an IR FSS nano-filter controlling the propagation of electromagnetic wave in a desired frequency band. An array of plasmonic tripods is studied as a frequency selective surface. By exploring the field distributions on the surface of the array, a circuit model is proposed. A strong coupling is introduced by putting two layers of plasmonic tripods close to each other. This strong coupling is characterized by a parallel LC circuit in the proposed model for the two layers of tripod. Then we utilize a filter theory concept where by cascading plasmonic resonant elements and controlling their locations a wideband performance is established. A nano-filter with stop-band characteristic in the frequency spectrum of 30THz to 85THz is demonstrated. A great agreement between the performance of the circuit model and the nano-filter is demonstrated. The independency of the nano-filter to the angle of incidence and polarization states for both TE and TM waves is successfully demonstrated.
Chapter 4

Multi-material loops; a promising building block for different applications

Introduction

The great attention to localized surface plasmon wave due to its astonishing optical property and wide variety of applications has broadened the researcher’s insight into this optical phenomenon in recent years [14, 67-72]. The plasmon wave is localized on the surface of sub-wavelength plasmonic particles at specific frequency that is dictated by the particle geometry and the optical properties of the material [29]. Sub-wavelength inclusions with different shapes are employed in order to fulfill the desired performance in different applications such as optical sensing, cloaking, high-resolution imaging, optical filtering, etc. [14, 58, 70, 72-74]. The excessive dependency of this resonance phenomenon on the sub-wavelength particle’s shape and the high intensity near field open up the possibility for bringing different sub-wavelength particles close to each other to provide novel physics [30-32, 70]. Also, recent advances in nano fabrication have made it more realistic to think about more complex structures to fulfill the desired performance. Nano-skiving has shown to be a capable method of fabricating concentric loops with different materials in a large-size array [34].

Based on the Mie theory, a sub-wavelength plasmonic sphere goes to resonance when its permittivity is around -2 [75]. Changing the aspect ratio of the particle can control the permittivity value at which the structure will provide resonance [29]. In other words, for any sub-wavelength plasmonic particle, based on its shape there will be a specific permittivity that makes the inclusion goes to resonance regardless of the plasmonic material (resonant permittivity). For an array of single plasmonic loops the radius, height and thickness of the loops play critical roles in defining the resonant permittivity [76]. Due to the field enhancement on the surface of the loops, the surrounding dielectric material would also affect the performance of the array. Multi-
material loop as the building block of a metasurface, consisting of number of concentric plasmonic loops with dielectric spacer layers, is one configuration that can be tuned by a large number of parameters. The concentric plasmonic loops can be designed to have the minimum coupling in order to have different resonances far apart from each other. On the other hand one can take advantage of a design in which the coupling between the loop nano-antennas is enhanced and therefore interesting features such as Fano resonance and field intensity enhancement can be obtained. In other words for the high-coupled design there are two resonances with totally different features, one a very high Q mode and the other a wideband radiating performance. Beside the fabrication feasibility, the large flexibility in tuning the performance of the multi-material loop array increase the motivation to investigate this unique design.

In this chapter, we investigate the performance of periodic array of multi-material loops by means of the powerful finite-difference time-domain (FDTD) technique. First we consider a general Drude model for the plasmonic material and obtain resonance characteristic of a metasurface in terms of the loop parameters. Based on the obtained resonant permittivity and the Drude model function we show how the resonant frequency would vary for different materials. These results are used to design two different configurations with respect to the coupling between the loops. The low-coupled multi-material loop metasurface can be interpreted as a frequency selective surface with multiple bands in the transmission spectrum. Four different designs are considered to investigate the resonance characteristics. In the first design by considering silver for the plasmonic loops material the procedure of designing low-coupled multi-material loop building block is shown. The effect of plasma damping factor on the resonance of the low-coupled design is illustrated by assuming gold as the inner loop material in the second design. Furthermore, changing the resonant frequency from short infrared to long infrared by choosing ITO and AZO for the plasmonic loop materials is investigated in the third design. The fourth design is showing the capability of this building block in producing three different bands within the spectrum by using three low-coupled concentric loop nano-antennas. We show how one can control the resonances by choosing each loop parameter properly. Moreover the field intensity enhancement on the surface of the loops is investigated. The other arrangement is highly coupled plasmonic
loops. In this configuration on the contrary with the low-coupled design each null or peak in the transmission or reflection performance is due to the near field interference of the concentric plasmonic loops. As a result the appearance of the dark and bright modes is shown. At the first resonance a large field intensity enhancement is shown that can be employed in order to enhance the nonlinear effects or the sensitivity of the performance to the surrounding media [39, 77, 78]. Interestingly, the second resonance has a very different feature offering a low-loss wideband phenomenon. The building block has a sub-wavelength size as well. Through the whole study by taking advantage of the hybridization model proposed by Nordlander in [33] the characteristic of each resonance is studied based on the induced dipole moment of each plasmonic loop. Effects of spacer layer permittivity and loss on the performance of the both designs are studied. At last but not least the performance of multi-material loop building block when the loops are not concentric is investigated.

**Array of single plasmonic loops as the simplest form of multi-material loops**

The metamaterial building block in this work, in general, is a multi-material loop consisting of a number of concentric plasmonic loops with dielectric spacer layer in between as shown in Figure 0.1(a). The spacer layer dielectric is assumed to be free space unless stated otherwise. Periodic array of this building block is investigated with the full wave analysis method of finite-difference time-domain (FDTD) technique. Perfectly matched layers and periodic boundary conditions are used to terminate the computation boundaries [19, 20]. The Yee cell size is considered 2.5nm for the designs with silver or gold and 13nm for the designs with ITO or AZO. This choice of cell size will make the effect of FDTD staircase meshing negligible in modeling the loop shape. The general Drude model of \( \varepsilon(\omega) = \varepsilon_\infty - \omega_p^2 / (\omega^2 - j\gamma_p\omega) \) is considered for the plasmonic materials in this investigation. The simplest configuration of the multi-material loops unit cell is a single plasmonic loop inside the free space. For the loop geometry there are three parameters that dictate the resonant permittivity; radius (a), height (h), and thickness (d) as shown in Figure 0.1(b). The values for these parameters should be in accordance with the plasma frequency of the plasmonic material. Therefore we normalize loop parameters
to the plasma wavelength of the general Drude model. In Figure 0.1(c) the transmission and reflection coefficients of a periodic array of single plasmonic loop nano-antenna is shown. The radius of the loop is \(0.91\lambda_p\), the height is \(0.145\lambda_p\) and the thickness is \(0.07\lambda_p\) (\(\lambda_p\) is the plasma wavelength of the plasmonic material). The unit cell size of the square array is \(2.175\lambda_p\). The loop is excited with a planewave with k-vector along the axis of the loop. A resonance occurs at \(f/f_p = 0.061\), which corresponds to the first dipolar mode excited on the surface of the loop. Note that the dimensions of the loop at the resonance are \(a = 0.05\lambda, d = 0.0045\lambda, \) and \(h = 0.009\lambda\) where \(\lambda\) is the resonant wavelength, which proves the sub-wavelength feature size of the elements. This is a purely electric resonance considering the fact that surface charges accumulate at both ends of the loop diameter parallel to the electric field excitation. The charge distribution on the surface of the loop at this resonant frequency shows the appearance of the dipole mode (inset of Figure 0.1(c)). Here the charge distribution on the surface of the loop is obtained with respect to the boundary conditions of normal displacement vector in equation (4.1).

\[
\hat{n} \cdot (\vec{D}_2 - \vec{D}_1) = \rho_s \tag{4.1}
\]

Figure 0.1: (a) Schematic diagram of the multi-material loops metasurface. The gray, yellow and cyan loops represent the plasmonic loop while the green and red loops represent the dielectric loops. (b) The parameters of the loop geometry. (c) The transmission and reflection coefficients for a single plasmonic loop metasurface. In the inset the charge distribution on the surface of the loop is shown for the excited dipole mode.
The aspect ratio of a loop defined as the ratio of its thickness to its radius \((d/a)\) is a parameter that can be engineered in order to control the resonant permittivity. Note that for \(d/a = 1\) as the upper limit of the aspect ratio the geometry is a disk rather than a loop. According to [29] for the disk geometry as long as \(2a/h \gg 1\), the change in the resonant permittivity is very small by changing the height of the disk. In Figure 0.2 the resonant permittivity of a periodic array of single plasmonic loop is shown as a function of the loop radius and its aspect ratio. To show the slight effect of height while the condition of \(2a/h \gg 1\) is satisfied, the study has been done for two different heights as shown in Figure 0.2(a) and (b). For the rest of the paper the height of the multi-material loops are considered \(0.145\lambda_p\).

![Figure 0.2: The resonant permittivity of a single plasmonic loop metasurface for two different heights of (a) \(0.145\lambda_p\) and (b) \(0.2175\lambda_p\). The horizontal axis is the aspect ratio of the loop and the vertical axis is the loop radius normalized to the plasma wavelength of the plasmonic material.](image)

In the above investigation we are just interested in finding the resonant permittivity to be able to find the resonant frequency for different materials. Due to the fact that the plasmonic loss does not affect much the location of the resonant frequency, we have assumed the damping factor to be zero in our simulations just for the results in Figure 0.2. The inverse of the Drude model formula with damping factor equal to zero is the frequency as a function of the permittivity as shown in equation (4.2). This equation gives us the approximate resonant frequency of the metasurface with respect to the
plasma frequency of the loops material. For different materials this frequency can be in different spectrum based on their plasma frequency. The more exact resonant frequency is derived from the full wave analysis after the loop parameters are chosen properly according to the design procedure.

\[ f_{\text{res}} = \frac{f_p}{\sqrt{\varepsilon_{\infty} - \varepsilon_{\text{res}}}} \] (4.2)

Knowing the resonant frequency of an array of single plasmonic loop for different materials will help us to design multi-material loop metasurface with different characteristics that will be discussed in more details in the following. Figure 0.3 show the resonant frequency for four different materials, silver (\(\omega_p = 1.36 \times 10^{16}, \gamma_p = 2.73 \times 10^{13}\)), gold (\(\omega_p = 1.30 \times 10^{16}, \gamma_p = 1.11 \times 10^{14}\)), ITO (\(\omega_p = 2.627 \times 10^{15}, \gamma_p = 2.39 \times 10^{14}\)), and AZO (\(\omega_p = 2.21 \times 10^{15}, \gamma_p = 1.91 \times 10^{14}\)) [54, 79]. According to each material’s plasma frequency, the range of the loop radius that has been swept in these Figures is different as well as the spectrum of the resonant frequency. Note that the unit cell size of the periodic array would change accordingly as well. As an example the unit cell size of the design with silver and ITO as the loop material is 300nm and 1.56\(\mu\)m, respectively. In the following based on the obtained results in this section we will design multi-material loop metasurfaces in two different categories, low-coupled and high-coupled. In order to have the most accurate results we will consider the complete Drude model including the damping factor for the plasmonic materials for the rest of the study.
Figure 0.3: The resonant frequency obtained by equation (4.2) and the data in Figure 0.2(a) for materials of (a) silver, (b) gold, (c) ITO, and (d) AZO. Note that in each Figure the geometry of the loop has scaled up to the plasma wavelength of the material including the radius, height and center to center distance on the array. The colorbar show the resonant frequency in THz unit.

**Low coupled multi-material loops**

The performance of a multi-material loop metasurface can be predicted to some extend based on the response of each loop in the building block. When the resonances of the single loop metasurfaces are far apart from each other in a sense that they do not overlap each other’s bandwidth, in the multi-material loop configuration (concentric loops) the coupling between the loops is small. Based on the results in Figure 0.3 one could design such configuration by choosing the radius and the thickness of each loop such that the resonant frequencies are apart from each other. For two concentric loops the parameters of each loop could be chosen from either one of the curves in Figure 0.3 or two of them. Note that the unit cell size of the array is a function of the plasma frequency.
of the loop material. As a result for each material the unit cell size would be different. On the other hand, a small perturbation in the unit cell size has a negligible effect on the first resonant frequency. Therefore, as long as the plasma frequencies of the chosen materials for the building block are close, one can use the results in Figure 0.3 to design a low-coupled structure with two different materials and consider the plasma frequency of either of the materials for defining the unit cell size.

The performance of four different metasurfaces with low coupling is shown in Figure 0.4. In the first design two plasmonic loops are made of silver. The radii of the outer and inner loops are 125nm and 75nm, respectively. The thickness of each loop is considered 10nm. According to Figure 0.3(a) the bigger loop resonates at around 134THz while the smaller loop resonates at around 225THz. The full wave simulation results of three metasurfaces of the outer loop, the inner loop and the concentric loops are shown in Figure 0.4(a). The obtained resonant frequencies of the outer and inner loops by FDTD are 133.9THz and 228THz, respectively, which are very close to the predicted resonant frequencies. The concentric loop metasurface has two separate resonances close to the resonance of the individual loop arrays. Clearly it is observed that the first resonance mostly comes from the outer loop resonance while the second resonance is mainly due to the inner loop resonance. Figure 0.4(b) shows the performance of a multi-material loop metasurface with two different materials. As long as the parameters are chosen properly for the two loops the concept would be the same. Here we consider silver for the outer loop with radius of 100nm and thickness of 10nm. The unit cell size is considered based on the plasma wavelength of the silver, which would be 300nm. According to Figure 0.3(a) the metasurface of this individual loop resonates at 176.5THz. The inner loop is assumed to be gold with radius of 60nm and thickness of 12.5nm to resonate at 298THz with respect to Figure 0.3(b). Due to higher loss of gold compared to silver, the resonance of gold is wider in bandwidth and less deep in amplitude. The obtained resonant frequencies of the outer loop and inner loop metasurfaces from FDTD are 176.8THz and 301.6THz, respectively. Again here we see a good agreement between the predicted resonant frequencies and the full wave simulation results. By using materials like ITO and AZO instead of silver and gold one would be able to bring down the resonant frequency of the metasurface from near and short infrared to mid and long infrared.
Figure 0.4(c) the performance of such design is shown. In this design outer loop is assumed to be ITO with radius of 624nm and thickness of 312nm. The metasurface of this ITO loop resonates at 62THz according to Figure 0.3(c). The full wave analysis result shows the resonant frequency to be at 61.7THz. For the inner loop the material is considered AZO with radius of 208nm and thickness of 156nm. The resonant frequency of this metasurface is 101THz from Figure 0.3(d) and 100.7THz from FDTD results. Due to the high loss of both ITO and AZO, the resonances of the single loop array are wide in bandwidth. This will force the designer to separate the two resonances more apart from each other at the first step when the parameters of the loops are chosen from Figure 0.3(c) and (d) to prevent the coupling between the two loops in the multi-material loop building block. Another beauty of this design is the capability of having three or more separate resonances by designing the concentric loops properly. Figure 0.4(d) illustrates the performance of three concentric loops made of sliver with radii of 125nm, 85nm and 40nm while the thickness of the three loops is 10nm. Based on the first assumption for the unit cell size of the periodic array and the height of the loops we consider $T = 2.175\lambda_p(\text{silver}) = 300\text{nm}$ and $h = 0.145\lambda_p(\text{silver}) = 20\text{nm}$ for the designs of Figure 0.4(a), (b), and (d) and $T = 2.175\lambda_p(\text{ITO}) = 1.56\mu\text{m}$ and $h = 0.145\lambda_p(\text{ITO}) = 104\text{nm}$ for the design in Figure 0.4(c). In order to reduce the effect of loss for the rest of the study we consider silver for the multi-material loop metasurface.
Figure 0.4: Transmission coefficient of four different multi-material loop metasurface designs with low coupling between the concentric loops. (a) Both loops are made of silver with radii of 125nm and 75nm for the outer and inner loop, respectively. The thickness of each loop is considered 10nm. (b) The outer loop with radius of 100nm and thickness of 10nm is considered silver while the inner loop with radius of 60nm and thickness of 12.5nm is assumed to be gold. (c) The multi-material loop metasurface made out of ITO for the outer loop with radius of 624nm and thickness of 312nm and AZO for the inner loop with radius of 208nm and thickness of 156nm. (d) The transmission coefficient of multi-material loop metasurface with three concentric silver loops. The radii are 125nm, 85nm, and 40nm and all the loops have the same thickness of 10nm. The red-dashed line shows the transmission coefficient for the array of outer loop and the blue dash-dotted line shows the transmission coefficient for the array of inner loop. For the design in part (d) the green line shows the transmission coefficient of the loop in between the outer and inner loops. Note that for the designs containing silver or gold the height of the loops are considered 20nm and the center to center distance between the multi-material loops are considered 300nm. For the designs with ITO or AZO the height is assumed to be 104nm and the center-to-center distance is 1.56µm.

Comparing the performance of single loops to multi-material loops with low coupling between the loops in Figure 0.4 illustrates that the first resonance in the two concentric loops design is narrower in bandwidth compared to the single outer loop resonance. At this resonance the dipole moments induced on each loop are anti-parallel as
shown by the surface charge distribution on the loops in Figure 0.5(a). Therefore, the net dipole moment decreases at this resonance and results in decreasing the bandwidth of the resonance. Compared to the outer loop metasurface, localized field intensity enhancement and larger sensitivity to the surrounding media permittivity are the consequences of the subradiant nature of this resonance. On the other hand the second resonance has a wider bandwidth compared to the single inner loop resonance. As shown in Figure 0.5(b) the parallel dipole moments of each loop will increase the net dipole moment of the second resonance. As a result the bandwidth of the resonance is enhanced and it has a superradiant character with lower field enhancement and lower sensitivity to the surrounding media compared to the single inner loop metasurface.

Figure 0.5: The charge distribution on the surface of the multi-material loop design corresponds to Figure 0.4(a) at two resonances (a) first resonance, and (b) second resonance.

High intensity localized field is a well-known characteristic of a sub-wavelength plasmonic particle resonance. Figure 0.6(a) and (c) are the field distribution at the first and second resonances of the low-coupled design in Figure 0.4(a), respectively. Here we compare the field distribution of the multi-material loop metasurface with an array of single plasmonic loop. Because the first resonance is due to the outer loop resonance and the second resonance comes from the inner loop, we compare Figure 0.6(a) to the field distribution of the array of outer loop in Figure 0.6(b) and Figure 0.6(c) is compared to the field distribution of the array of inner loop in Figure 0.6(d). The electric field intensity is calculated in the plane perpendicular to the axis of the loop and at the middle
of the loop’s height. According to the low coupling of the two concentric loops at the first resonance the field is mostly localized on the outer loop while at the second resonance the inner loop surface has the localized field on itself. The subradiant character of the first resonance can be observed here in the higher field localization at the first resonance compared to the single outer loop array. Also the lower electric field localization at the second resonance compared to the inner loop array is an evidence for the superradiant characteristic of the second resonance.

![Electric field intensity distribution for (a) multi-material loop metasurface of design in Figure 0.4(a) at the first resonance, (b) single outer loop metasurface at its resonance, (c) multi-material loop metasurface at the second resonance, and (d) single inner loop metasurface at its resonance. The dashed lines show the boundary of the plasmonic loops. The colorbar show the electric field intensity in (V/m)^2.](image)

Figure 0.6: The electric field intensity distribution for (a) multi-material loop metasurface of design in Figure 0.4(a) at the first resonance, (b) single outer loop metasurface at its resonance, (c) multi-material loop metasurface at the second resonance, and (d) single inner loop metasurface at its resonance. The dashed lines show the boundary of the plasmonic loops. The colorbar show the electric field intensity in (V/m)^2.
High coupled multi-material loops

As long as the coupling between the loops are small each resonant can be controlled by changing the corresponding loop’s aspect ratio. From Figure 0.3 we can see that by increasing the aspect ratio of the loop the resonant frequency will have a blue shift. Now consider that we fix the inner loop geometry and start to increase the aspect ratio of the outer loop by increasing its thickness. If the blue shift of the first resonance is large enough so that the second resonance happens to be in the bandwidth of the first resonance then the prerequisite of Fano resonance is achieved. This will enhance the coupling between the two loops dramatically and result in appearance of a dark mode with vanishing net dipole moment and a bright mode with superradiant characteristic that has radiating wideband profile [30-32, 70, 80, 81]. In order to design high-coupled multi-material loop metasurface, using Figure 0.3, the geometry of the two loop nano-antennas will be chosen such that the resonant frequencies of the individual loop array are close to each other. In contrast with the low-coupled multi-material loops here the resonances of the multi-material loop metasurface do not resemble the resonance of each loop but they are based on the near field interaction of the concentric loops. We consider two loops of silver with radii of 125nm and 75nm and thickness of 30nm and 10nm for the outer and inner loops, respectively. The two arrays of the outer and inner loops resonate at 215THz and 225THz, respectively. The transmission coefficient of the multi-material loop metasurface as well as each individual loop array is shown in Figure 0.7(a). In the transmission coefficient there are two null and a sharp peak in between which is labeled by (I), (II), and (III). The charge distribution at each of these resonances (as shown in Figure 0.7(b)-(d)) along with the net dipole moment calculated from equation (4.3) can help us to better understand the characteristics of each of these three frequencies.

\[
\vec{P}(\vec{r}) = \int_{V} \rho(\vec{r}_0)(\vec{r}_0 - \vec{r})d^3\vec{r}_0
\]  

(4.3)

At the first transmission null labeled by (I) likewise the first resonance of the low-coupled design, the induced dipole moments on the loops are anti-parallel. The difference here is that the inner loop dipole moment reduces the net dipole moment more significantly compared to the low-coupled design. By moving toward higher frequency
the amplitude of the inner and outer loop dipole moment becomes closer while they are still antiparallel. As a result the dark mode (II) with almost zero net dipole moment appears between the two nulls in the transmission coefficient (the wave can pass through). High field intensity and large sensitivity to the surrounding media are two big characteristics of these two frequencies due to their subradiant nature. The second null in transmission coefficient or the bright mode (III) has a wideband feature due to the fact that the dipole moments induced on the surfaces of the outer and inner loops are in parallel. This is a very unique feature. The superradiant characters such as low field enhancement and high scattering are attached to this resonance. It must be mentioned that at all three modes the building block has a sub-wavelength size.

Figure 0.7: Performance of multi-material loop metasurface with high coupling between the loops. (a) The transmission coefficient of the multi-material loop (solid line), the outer loop (dashed
line), and the inner loop (dashed-dotted line). Parts (b) to (d) show the charge distribution of
frequencies (I), (II), and (III), respectively. At each of these Figs. the pink (left) arrows show the
dipole moment of inner loop, the green (right) arrows show the dipole moment of the outer loop and
the orange (center) arrows show the net dipole moment of the multi-material loop building block.

Taking advantage of the high coupling between the loops can considerably enhance
the localized electric field intensity. For the design in Figure 0.7 the electric field
intensity distributions at three frequencies of (I), (II), and (III) are shown in Figure 0.8
both in (V/m)² and dB. Figure 0.8(a) and (d) show the electric field intensity distribution
at frequency (I). At this subradiant mode the electric field is mostly confined within the
spacer layer due to the antiparallel dipole moments of the inner and outer loops. Moreover, there is some field localization on the external surface of the outer loop with
lower intensity because of the non-vanishing net dipole moment at this frequency. The
electric field intensity distribution at frequency (II) can be seen in Figure 0.8(b) and (e).
At this frequency the field is just confined within the spacer layer with no field outside of
the outer loop. This behavior can be explained by the zero net dipole moment at this
frequency. Considering the small volume and the very large intensity of the electric field
this can be used to enhance the nonlinear effects. Also this results in more sensitivity to
the spacer layer permittivity that can be used in optical sensing. Moreover, according to
the high transmission coefficient at this frequency the energy is transmitted through the
spacer layer and electromagnetically induced transparency can be achieved [82]. On the
other hand, at frequency (III) the field is localized mostly on the surface of the outer loop
(Figure 0.8(c) and (f)) and according to the superradiant characteristic of this resonance,
the intensity of the localized field is much lower than in the other two frequencies. This is
in fact the main reason for having a wideband performance at this frequency (shown in
Figure 0.7(a)).
Figure 0.8: The electric field intensity distribution at three frequencies labeled by (I) to (III) in Figure 0.7 are shown in (V/m)\(^2\) in parts (a) to (c) and in dB in parts (d) to (f), respectively. Note that the Figs. in dB unit are normalized to the maximum value of the field intensity in parts (a) to (c).

**Effect of spacer layer permittivity and loss**

In multi-material loop design one can use a proper dielectric material between the plasmonic loop nano-antennas to control the resonance characteristics in desired ways. Resonances with high quality factor exhibit more sensitivity to the perturbations compared to low quality factor resonances. On the other hand, the permittivity of the spacer layer is much more effective in changing the resonant frequency if the field is localized within the spacer layer. As a result the high-coupled multi-material loop metasurface should undergo more significant changes compared to the low-coupled design for a same amount of perturbation in the spacer layer permittivity. Also for the high-coupled design due to the fact that the field is localized within the spacer layer at the first null (I) and the first peak (II) in transmission coefficient, these two frequencies are much more sensitive to the spacer layer permittivity than the second null (III) in the transmission coefficient. In order to show these effects, the spacer layer permittivity is swept between 1 to 4 in our simulations for the two designs in Figure 0.4(a) (low-coupled) and Figure 0.7 (high-coupled). For the low-coupled design, as illustrated in
Figure 0.9(a), both resonances experience red shifts. We have fitted a line on the change in first and second resonance frequency versus the spacer layer permittivity (Figure 0.9(b)). The slopes of both lines are close to each other. For the high-coupled case (shown in Figure 0.9(c)) the first null (I) and the peak (II) experience significant changes due to both high quality factor of the resonance and also the localization of the fields within the spacer dielectric layer. The slope of the change in resonant frequency (I) versus the spacer layer permittivity is twice of that for the low-coupled case. In contrary, the frequency of the second null (III) does not change considerably by perturbing the spacer layer permittivity due to the superradiant character and also the weak field intensity within the spacer layer.

The absorption performance of the system is also studied. We consider two cases for the permittivity of spacer layer, $\varepsilon_r = 2 + j0.02$ and $\varepsilon_r = 2 + j0.2$. The results for low and high coupled cases are shown in Figure 0.9(e) and (f), respectively. Increasing the loss of the spacer will increase the absorption in the system, unless for the second transmission null for the high-coupled case. This is a very interesting phenomenon indeed as the loss at this frequency is small in comparison to all other designs. Namely, for the resonances that there are strong localized fields within the spacer layer the loss in permittivity will affect the absorption greatly. But for the second null of high-coupled case the field is not localized and as such the design is not sensitive to the loss. As a result we have a subwavelength building block with wideband and low loss characteristics. The beauty of the high-coupled design is that there are two resonance phenomena with totally different characteristics. At the first resonance, which is characterized as subradiant; by changing the spacer layer permittivity from 1 to 2 according to Figure 0.9(c), the first resonant frequency is changing from 165THz to 142THz. Consequently, the transmission coefficient at 165THz is changing from 92% to 22% that makes the design an ideal candidate for sensing applications. On the other hand the second resonance has a wide bandwidth with low loss due to its superradiant character.
Figure 0.9: The effect of spacer layer permittivity and loss on the resonances of the multi-material metasurface. (a) The transmission coefficient of the low-coupled multi-material loop metasurface design. (b) First and second resonant frequencies versus the spacer layer permittivity. (c) The transmission coefficient of the high-coupled multi-material loop metasurface design. (d) Change in the frequencies of the two nulls in the transmission coefficient versus the spacer layer permittivity. The dashed lines in parts (b) and (d) are the fitted line on the data. The absorption of the metasurface for (e) low-coupled and (f) high-coupled designs. In the two later figures the permittivity of the spacer layer is assumed to be $\varepsilon_r = 2 + j0.02$ for blue-solid curve and $\varepsilon_r = 2 + j0.2$ for red-dashed curve.
**Effect of breaking the symmetry**

For many applications like sensing and nonlinear optics, high field intensity is desired. For the sensing this will result in more sensitivity to the surrounding media and for nonlinear optics the nonlinear effects are increased. In the previous sections it was shown that by increasing the coupling between the dipolar modes of the concentric loops, the field is concentrated within the spacer layer with a high intensity. Another way to enhance the field intensity is to break the symmetry. Breaking the symmetry will result in appearance of the higher order multi-polar modes. Taking advantage of these new modes, a tunable Fano like resonance can be achieved [30]. To investigate these effects, the design in Figure 0.4(a) is considered while the inner loop has an offset in two directions; parallel to the incident electric field, z direction, and perpendicular to the incident electric field, y direction as shown in the inset of Figure 0.10. Breaking the symmetry in either direction has introduced another resonant feature to the transmission spectrum. Comparing the response of the concentric loops and the one with 30nm offset can clearly show that the resonance of the inner loop (second resonance) is coupled to another resonance and result in lower and higher energy resonances. This can be verified by obtaining the charge distribution at each of these resonances. Increasing offset in either direction result in obtaining a stronger Fano-like resonance.

![Figure 0.10: The transmission coefficient for non-concentric loops. The inner loop center has an offset (a) parallel and (b) perpendicular to incident electric field direction.](image)

In order to characterize each of the resonances, the charge distribution on the surface of the loops should be obtained according to equation (4.1). Figure 0.11 shows the charge
distribution on the surface of the loops when the inner loop center has an offset of 30nm in the direction of incident electric field. For the first resonance, likewise the concentric loops, each loop has dipole moments which are anti-parallel to each other. Interestingly, for the second and third resonance we see the appearance of quadrupole mode on the outer loop. Note that the quadrupole mode cannot be excited with normal planewave incidence on a loop due to the zero net dipole moment. However, breaking the symmetry causes the excitation of this magnetic dipolar mode. This mode happens to be in the bandwidth of the inner loop resonance. Having a narrowband resonance (outer loop quadrupolar mode) within the wideband resonance (inner loop dipolar mode) will result in a Fano like resonance as can be seen in Figure 0.10(a).

![Figure 0.11](image1.png)

**Figure 0.11:** The charge distribution on the surface of the non-concentric loops at (a) 120THz, (b) 216THz, and (c) 270THz. The offset of 30nm is parallel to the incident electric field direction.

The same study is done for the case when the 30nm offset is perpendicular to the incident electric field direction. For the first resonance, the dipolar modes of each loop are excited and they are anti-parallel. For the second and third resonances, the quadrupolar mode is excited on the outer loop while the inner loop has a dipolar mode. For both directions of the offset, the dipole moments of the outer and inner loops at the second and third resonance are parallel to each other. Figure 0.12 shows the charge distribution for the three resonances of the multi-material loops when the offset of the inner loop is perpendicular to the incident electric field.
Figure 0.12: The charge distribution on the surface of the non-concentric loops at (a) 123THz, (b) 211THz, and (c) 250THz. The offset of 30nm is perpendicular to the incident electric field direction.

One of the consequences of breaking the symmetry is increment in the intensity of the localized electric field. Note that the design we are investigating in this section is a low coupled design when the loops are concentric. As shown in Figure 0.6, although the first resonance has a sub-radiant character, the field intensity does not exceed $750(V/m)^2$ due to the low coupling of the loops. In other words, because of the distance between the charges of opposite sign on the inner and outer loops, the field enhancement is limited. Also because of the super-radiant characteristics of the second resonance high field intensity is not expected. The field intensity distribution for the cases with offset in either direction is shown in Figure 0.12. For the offset in the direction of electric field, at the first and second resonances we see a huge field enhancement compared to the concentric loops. Notice the charge distribution in Figure 0.11(a) and (b). In the region where the inner loop is very close to the outer, the charges on the loops have an opposite sign with respect to each other. This can explain the field enhancement for the first two resonances. However, this is not the case for the third resonance and the charge distribution shown in Figure 0.11(c) can verify the lower field enhancement at this resonance. On the other hand, for the case with offset perpendicular to the electric field direction, the field enhancement at the first resonance is similar to the concentric loops. The charges of opposite sign are further away from each other compared to the case with offset in the z direction. As a result we see less intensity in the localized electric field. The same reasoning is valid for the third resonance. At the second resonance, we see opposite sign charges accumulated on each loop where the inner and outer loops are close to each other, and that is the reason for higher field intensity at the second resonance. In general...
we can have this rule of thumb that when the charges of opposite sign get close to each other, it can result in high field intensity. This general rule can explain why we get high field enhancement for the high coupled design, and non-concentric loops.

Figure 0.13: The electric field intensity distribution at (a) 120THz, (b) 216THz, and (c) 270THz for the case with offset of 30nm in the direction of incident electric field, and (d) 123THz, (e) 211THz, and (f) 250THz when the offset of 30nm is perpendicular to the incident electric field.

Conclusion

The performance of single plasmonic loop array is employed to obtain a recipe for designing multi-material loop metasurfaces with low and high coupling between the concentric loop nano-antennas. For the low-coupled multi-material loop metasurface the parameters of the loops are chosen such that their resonant frequencies are far apart from each other. Four different designs are proposed; in the first design the two loops are considered silver and in the second design by considering gold as the inner loop the effect of higher plasma damping factor is shown. In the third design by changing the material of the loops from silver and gold to ITO and AZO with lower plasma frequency we show the ability of bringing the resonant frequency down from short infrared to long infrared. It is noteworthy that the dimensions in each design are directly related to the plasma frequency of the materials used in the building block. The fourth design shows another
great capability of this building block to have three resonances that are not coupled to each other and they can be controlled by the aspect ratio of the three concentric loops in the building block. Although the coupling between the loops here is small, the subradiant and superradiant characters of each resonance are revealed by the induced dipole moments on each loop. The high coupling is achieved by bringing the resonance of the loops close together. Unique resonance characteristics including Fano-like feature are demonstrated. Taking advantage of the hybridization model the characteristics of different resonances are studied based on the induced net dipole moments. The appearance of the dark mode is illustrated by showing the equal but antiparallel dipole moments of the inner and outer loops. The sensitivity of the performance of both designs to the spacer layer permittivity and loss is studied as well. The effects of breaking the symmetry in the multi-material loop building block, which are exciting the quadrupolar mode of the loop and electric field intensity enhancement, are also studied. It is shown that for the high-coupled design there are two resonances with completely different characteristics. One is narrow in bandwidth with large field enhancement and extremely sensitive to the spacer layer material. The other resonance phenomenon has a wide bandwidth with low loss. The building block at both frequencies is sub-wavelength ($\lambda/7$ and $\lambda/5$, respectively). The first resonance can be integrated for near field applications such as sensing and nonlinear optics, while the second resonance can be used for making wideband low-loss metamaterials. The multi-material loop building block provides great opportunity in design space where one can tailor very unique optical features by controlling the aspect ratio of each loop and their couplings.
Chapter 5

Engineering optical bistability in multi-material loop metasurface

Introduction

Optical nonlinearity is the essential platform in all optical signal processing, creation of ultra-short pulses, quantum information applications, and ultrafast switching [25, 35, 83]. All optical switching as one of the basic elements of any signal processing unit can be achieved by employing different optical nonlinear effects such as Kerr effect [35]. In general the optical properties of materials depend on different characteristics of the incoming light including but not limited to the light intensity. Kerr effect is a change in the refractive index of a material due to the applied electric field intensity (equation (5.1)) [83]. Adding a feedback mechanism to the Kerr effect such as resonance phenomenon, results in appearance of optical bistability. The output of system with optical bistability has two distinguished steady states for an identical input. In other words, the output depends not only on the current state of the input but also on its previous state as well [84, 85]. Optical memory, optical transistor, and all optical logic gates are some of the optical bistability applications that has been investigated by researchers [78, 86, 87].

\[ \varepsilon_{NL} = \varepsilon_L + \chi^{(1)}|E|^2 \]  

(5.1)

Kerr effect likewise other optical nonlinear effects is essentially weak due to its principal mechanism of photon-photon interaction [35]. A system, which enhances the electric field intensity within the nonlinear material, is of great interest. On the other hand, high sensitivity of a resonance to the dielectric properties of the surrounding medium is desired for employing Kerr effect in optical switching, because by small perturbation in the dielectric constant of the surrounding material the resonant frequency of the structure is disturbed. As a result by increasing the intensity within the nonlinear material the scattering from the resonating particle will change significantly. This
sensitivity can be quantified with the quality factor of the resonance. A resonance with high quality factor is highly dependent on the surrounding medium characteristics. These two characteristics are the well-known properties of localized surface plasmon (LSP) resonance. The coherent oscillation of the conduction electrons on the surface of a subwavelength plasmonic particle due to an external electric field, i.e. the localized surface plasmon resonance, will result in high field intensity in the near field region of the plasmonic particle. Also the LSP resonance is highly sensitive to the surrounding medium’s dielectric characteristics. This can explain the huge attention to the nonlinear plasmonics in recent years; surface plasmon propagation as well as localized surface plasmon are used to achieve nonlinear directional coupler, optical switching in metal-slit arrays and gratings, nonlinear optical antennas, and programmable photonic components [38, 77, 88-94].

In multi-material loop (MML) metasurface both high field intensity and great sensitivity to the spacer layer dielectric are achievable by engineering the coupling between the loops. In our recent study we show that by increasing the coupling between the plasmonic loops, the field can be confined within the spacer layer with huge field intensity. Furthermore, due to the subradiant nature of the first resonance in the high coupled MML metasurface, this resonant frequency is highly dependent on the spacer layer material’s permittivity [95]. Taking advantage of these two features in MML building block, we investigate the optical bistability in this metasurface by integrating Kerr nonlinear material within the spacer layer. Through this study we use finite difference time domain (FDTD) technique. The Kerr nonlinearity is implemented in the Yee’s algorithm by solving the nonlinear equation between the displacement (D) and electric field (E) vectors with Newton iteration technique [96, 97]. Periodic boundary condition as well as perfectly absorbing boundary condition is used to terminate the computational domain [19]. Effects of engineering the coupling between the loops on the bi-stable behavior of the metasurface are explored comprehensively.

**Optical bistability in MML Metasurface**

The building block of MML metasurface consists of two concentric plasmonic loops with a nonlinear material as the spacer layer (depicted in Figure 0.1). Silver is used as the
plasmonic material of the loops with Drude model for its permittivity. The plasma frequency of the silver is considered 2175THz and the damping factor is 4.35THz [54]. For the nonlinear material we use data found in literature for InGaAsP with linear permittivity of $\varepsilon_L = 2.25$ and the third order susceptibility of $\chi^{(3)} = 10^{-9}(m^2/V^2)$ [88]. The periodic structure under investigation has a period of 300nm. The parameters depicted in Figure 0.1(a) are as follow: $R_1=125nm$, $R_2 = 95nm$, $R_3=75nm$, $R_4=65nm$, and $H=20nm$ (H is the height of the loops). The transmission coefficient versus frequency is depicted in Figure 0.1(b). The first resonance is of subradiant nature with a higher quality factor compared to the second resonance. In addition, the field distribution at the first resonance elucidates highly confined electric field within the spacer layer in the contrary with the second resonance. The electric field distributions at these two resonances are shown in Figure 0.1(c) and (d). The large quality factor and high field enhancement at the first resonance compared to the second one are the reasons that we put our focus in this study on the first resonance of this metasurface for obtaining the optical bistability.

![Figure 0.1](image1.png)

Figure 0.1: (a) The schematic of the multi-material loop metasurface building block. (b) The transmission coefficient of the metasurface with parameters of $R_1=125nm$, $R_2 = 95nm$, $R_3=75nm$, $R_4=65nm$, and $H=20nm$. The electric field distribution at two resonances at (c) 125THz and (d) 245THz.
Kerr effect in addition to a feedback mechanism is required to obtain optical bistability. The Kerr effect is integrated into this metasurface by assuming a Kerr nonlinear material for the spacer layer and the resonance itself is the feedback mechanism. It is required that the condition of equation (5.2) between the resonant frequency \( \omega_{\text{res}} \), the incident light frequency \( \omega_0 \), and the decay rate of the resonance \( \gamma \) is satisfied to obtain a bi-stable behavior. Increasing the incident light intensity causes a redshift in the resonant frequency. As the resonant frequency moves toward the incident light frequency due to increasing the incident light intensity, the field enhancement within the spacer layer is increasing as well and the positive feedback mechanism is achieved. After reaching the required incident intensity these two frequencies overlap and the metasurface goes to resonance state and the transmission coefficient drops to a lower value. On the other hand, decreasing the incident light intensity after the metasurface reaches the resonance will cause the resonant frequency of the metasurface to go back to its initial value. However, because of the large quality factor of this resonance the decay rate is very small and the resonator tends to keep the energy inside itself. Therefore, due to the negative feedback mechanism it is possible to keep the resonator in its resonance state by smaller input intensities after it reaches the resonance. So by decreasing the incident light intensity the transmission stays in a lower value for intensities smaller than the required intensity to make the metasurface go to resonance and optical bistability is achieved.

\[
\frac{\omega_{\text{res}} - \omega_0}{\gamma} > \sqrt{3}
\]

(5.2)

To obtain the optical bistability by means of FDTD the amplitude of the incident planewave should increase gradually to its maximum and then decrease with the same slope. This gradual change or the long pulse width is necessary to make sure the obtained curve is representing the steady state output for different amplitudes. The electric field is considered as a saw-tooth function modulated with a sinusoidal function as in equation (5.3).
where $E_0$ is the maximum input intensity, $\omega_0$ is the modulating frequency, and $T$ is the input pulse width. For the configuration under study the resonant frequency is around 125THz. The metasurface is excited with a planewave propagating along the axis of the loop and electric field polarized along the diameter of the loops with frequency of 116THz. In the linear state (low incident intensity) at the resonance 20% of the incident light transmitted to the other side of the metasurface while at 116THz the transmitted light is about 78% of the incident light. The envelopes of the incident pulse as well as the transmitted signal are depicted in Figure 0.2. It is clear that after reaching certain incident amplitude, the transmission is switched to a lower value. This required amplitude is a function of the field enhancement within the spacer layer. Increasing the field enhancement will decrease this required amplitude. After the incident intensity reaches its maximum and starts to decay, the transmission coefficient stays in its lower value even when the incident light intensity drops below the required intensity for switching. At some specific input intensity (smaller than the required intensity for switching) the transmission coefficient will switch back to its initial value. As a result for the input intensities within these two specific values, the output has two stable states depending on the previous condition of the resonator.
The transmitted light intensity versus the incident intensity reveals the bi-stable behavior shown in Figure 0.3. The transmitted light intensity is around 78% when the incident light is weak. Increasing the input intensity beyond 1.7E15 (V²/m²) result in the overlap of the resonant frequency with the incident light frequency which is 116 THz. As a result the transmitted light intensity is dropped to a lower value. The transmission stays in the lower value while the input intensity is decreasing until it reaches 8.75E14 (V²/m²). Below this intensity, the metasurface is not resonating anymore and as a result the output intensity switches back to its high value. The input pulse width (T in equation (5.2)) is increased till the convergence is achieved as elucidated in Figure 0.3.

![Image](image.png)

Figure 0.3: The obtained bistability curve for three different pulse widths of 10ps, 20ps and 30ps. The convergence is achieved by the 30ps pulse width.

**Improving the extinction ratio**

High field intensity within the spacer layer leads to enhancement of spacer layer permittivity due to the Kerr effect. The increment of spacer layer permittivity has two effects on the transmission spectrum of a high coupled MML metasurface. First, the subradiant resonance experiences a redshift. Second, the amplitude of the transmission coefficient at this resonance is increased to a higher value (note that at the resonance most of the light reflected from the metasurface) [95]. As an example, in Figure 0.4(a) the transmission coefficient of the MML metasurface under investigation is shown for the spacer layer permittivity of 2.25 with the blue curve and that of 3.5 with dashed red line.
The transmission coefficient is increased from about 20% to 33%. Therefore, in the bistability curve, the transmission coefficient in the lower state is always higher than the transmission coefficient at the resonance in the linear state. One of the figures of merit for a switch is the extinction ratio defined as the ratio of the output intensity in the two states of ON and OFF. In order to increase the extinction ratio the transmission amplitude at resonance in the linear state should be small enough. This small transmission amplitude is achieved by decreasing the coupling between the plasmonic loops (increasing $R_2$). The blue triangles in Figure 0.4(b) show the amplitude of the transmission coefficient at the resonance for three different values of $R_2$. A reduction in the coupling makes the amplitude of the transmission coefficient closer to zero. Although this value enlarges by employing Kerr effect; the extinction ratio increases due to a smaller value of the initial transmission coefficient in the linear state. The cost of this increase in the extinction ratio is the higher required intensity to switch to the lower output intensity state. The drop in the enhancement of electric field intensity within the spacer layer due to lessening of the coupling explains the higher required intensity for switching. The maximum field enhancement within the spacer layer is shown with green rectangles in Figure 0.4(b) for the three values of $R_2$.

![Figure 0.4](image)

Figure 0.4: (a) Transmission coefficient for two values for spacer layer permittivity. The blue curve is for $\varepsilon_r = 2.25$ and the red curve is for $\varepsilon_r = 3.5$. (b) The triangles show the transmission amplitude at the resonance and the rectangles show the maximum field enhancement at the first resonance for different values of $R_2$ between 95nm and 105nm.

The bi-stable behavior of the MML metasurface is a function of the coupling between the plasmonic loops. For the low coupled design, the MML’s transmission spectrum does not change by increasing the incident amplitude because of the weak field enhancement within the spacer layer. On the other hand the subradiant resonance in the
high coupled design (first resonance) undergoes a significant change by increasing the incident light intensity. Higher coupling between the plasmonic loops leads to higher field enhancement within the spacer layer thus lower required intensity for switching from the high intensity output to the lower state. However, increasing the coupling lessens the extinction ratio of the two states due to the higher transmission amplitude at the resonance. Consequently, there is a trade-off between the required input intensity for switching and the extinction ratio of the switch. To elucidate this trade-off, a second design with \( R_2 = 105 \text{nm} \) is investigated. In Figure 0.4(b) it is shown that for this design the field enhancement as well as the transmission coefficient at the resonance are smaller than that of the first design (\( R_2 = 95 \text{nm} \)). The resonant frequency of this structure is around 127THz. The modulation frequency of the saw-tooth function in equation (5.3) is 110THz. This frequency is chosen so that the condition in equation (5.2) is satisfied and also the initial transmission coefficient of the metasurface is close to the first design which is around 78%. This way we can compare the extinction ratio with better accuracy. The bistability curve for this design is depicted in Figure 0.5. The required incident intensity for switching to the lower transmission coefficient is \( 2.3 \times 10^{16} \text{ V}^2/\text{m}^2 \) for the later design which is 13 times larger than that of the first design. On the other hand the transmission coefficient in the lower state is around 25% which makes the extinction ratio doubled compared to the first design.

![Bistability curve for the design with \( R_2 = 105 \text{nm} \). The coupling between the plasmonic loops is decreased. Hence the required input intensity for switching is 13 times higher compared to the design with \( R_2 = 95 \text{nm} \). However, the extinction ratio is doubled.](image)

Figure 0.5: Bistability curve for the design with \( R_2 = 105 \text{nm} \). The coupling between the plasmonic loops is decreased. Hence the required input intensity for switching is 13 times higher compared to the design with \( R_2 = 95 \text{nm} \). However, the extinction ratio is doubled.
Conclusion

In summary, we employed the Kerr effect in multi-material loop building block by assuming the spacer layer as a Kerr nonlinear material. The optical bistability is obtained by means of nonlinear finite difference time domain method. The input intensity has a saw-tooth profile to be able to increase and decrease the incident amplitude. The effects of coupling between the plasmonic loops on the optical bistability curve are studied comprehensively. By engineering the coupling between the loops the extinction ratio between the two states of output is increased by a factor of 2. At the same time due to lower field enhancement, the required input intensity is 13 times higher than that of the first design.
Chapter 6

Recommendations for Future Works

The science of plasmonic metasurfaces is one of the hottest topics of research in the metamaterial community. Transmitarray metasurfaces can be designed for beam steering as well as beam focusing or in more general way, for light manipulation. Controlling the polarization of the transmitted light is a practical feature that can be added to the functionality of a transmitarray metasurface. Also the bandwidth of the transmitarray is another point of interest that can be addressed in future works. On the other hand, integrating nonlinearity with plasmonic metasurfaces opens up a wide range of possibilities for all optical signal processing, quantum computing and all optical switching. Different geometries can be studied in order to optimize the switching parameters such as extinction ratio and the minimum required input intensity for switching. Moreover, integrating Kerr effect with surface plasmon polariton wave-guiding mechanism is another promising path for future research to design all optical switches and all optical logic gates. Recent advances in characterizing and fabricating the one atom thick layer of Graphene has shown the Graphene as a promising platform for optical nonlinearities due to its low loss as well as controllable conductivity.
References


[34] D. J. Lipomi, M. A. Kats, P. Kim, S. H. Kang, J. Aizenberg, F. Capasso, *et al.*, "Fabrication and replication of arrays of single or multicomponent nanostructures..."


List of Publications

**Journal Papers**


**Conference Papers**

Jongbum Kim, Babak Memarzadeh, Aveek Dutta, Sajid M. Choudhury, Alexander V. Kildishev, Hossein Mosallaei, and Alexandra Boltasseva, “GZO/ZnO Multilayered nanodisk metasurface to engineer the plasma frequency”, submitted to CLEO, San Jose, CA, USA, June 8-13, 2014.


