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Inducing multiple Fano resonant modes in split concentric nanoring resonator dimers for ultraprecise sensing

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Abstract
We report on finite-difference time domain analysis of silicon split concentric ring resonator dimers (SCRRDs) with nanoscale dimensions deposited on a dielectric substrate to design all-dielectric polarization-dependent metamaterial (MM) structures. Investigating the optical response of an SCRRD on a quartz (SiO₂) substrate, we verified that it can be considered as a meta-atom to design a MM. The proposed structure is able to support double sharp Fano resonances in the visible spectrum under transverse electric polarization excitation. Immersing the all-dielectric MM in various chemical liquids with different refractive indices and calculating the transmission spectra, we estimated the sensitivity of the presented MM as 497 nm/RIU and the corresponding figure of merit as 118.5. This study could help designing ultra-sensitive, low-cost and efficient bio-chemical sensors based on all-dielectric components.

Keywords: split ring resonator, dimer, metamaterial, Fano resonance, FOM, FDTD

1. Introduction

All-dielectric subwavelength components and structures have a great potential to be used in designing numerous types of metamaterials (MMs) with a wide range of applications including but not limited to ultra-sensitive bio-chemical sensors, light emitters, light velocity reducers, nanoantennas, and second harmonic generation grating structures [1–5]. Unlike natural materials, the optical properties of MMs are not essentially determined by their chemical composition, but rather by the shape, size and structural design of their unit cell which is often called as ‘meta-atom’ and also distribution of these meta-atoms in ‘meta-molecules’ and MM lattice [6]. These features enable tailoring ultrasensitive nanoscale sensors with high figure of merits (FOMs) and quality factors to detect subtle environmental perturbations in the environmental conditions [7]. In addition, it is shown that these structures could also be tailored to support strong Fano resonance (FR) modes from visible to near infrared region that are resulted from destructive interference between dark and bright modes in a particle system in molecular levels [8, 9]. Due to the absence of strong lossy components in dielectric-based molecular structures, destructive and weak interference between dipolar and quadrupolar dark and bright resonant modes can result pronounced FR dips in the extinction profile [9, 10]. On the other hand, closely packed dielectric nanoparticles (NPs) have been considered as molecular structures that are able to support strong magnetic dark and bright modes in a finite oligomer-type system, and the result of this scenario is the formation of FRs in the spectral response of the structure [10, 11]. The complexity, symmetry, and orientation of employed dielectric or semiconductor NPs have significant impacts on behavior, sharpness, narrowness, depth, position, and even number of FR dips. Miroshnichenko et al [11] has proved that pronounced FR dips can be induced in silicon-based antisymmetric and heterogenous oligomer nanoclusters in the visible wavelengths, where these resonances originate from the magnetic dipole resonant modes correlated to each one of individual NPs with high refractive indices coupled to electrical dipolar resonant modes around NPs. In terms of theoretical analysis, Mie scattering theory has been widely utilized to describe the behavior of silicon-based NP clusters and also to specify the interaction between bright and dark magnetic dipole resonant
modes inside the NP systems [12]. It is well-accepted that in an individual dielectric NP, a constructive interference between the excited magnetic dipole modes and the opposite polarization of the electric field on the other side of the particle gives rise to appearance of bright resonant modes [11, 13].

Inducing pronounced FR dips with high qualities in simple and symmetric metallic (plasmonic) molecular clusters have been studied extensively in the past due to their high performance in practical applications [14–17]. In terms of structural orientation, among molecular NP clusters, homogeneous ‘dimer’ has been considered as one of the simplest molecular structures, which is composed of a couple of equivalent NPs that are placed a few nanometers from each other as an offset gap distance [18, 19]. The major problem regarding dimer (with metallic or dielectric NPs) is the absence of structural complexity and antisymmetry that are required to excite and induce new dark resonant modes in single or collective regimes. Very recently, heterogeneous bimetallic dimers are proposed to support Fano-like and Fano resonant modes in certain bandwidths [20, 21]. However, FRs in dimer-type structures have relatively poor quality compared to the ones in highly complex clusters since excitation of strong dark resonant modes is challenging in metallic and dielectric dimer colloids. To induce very strong dark modes in a silicon-based dimer structure, we proposed a complex dimer composed of dielectric NPs with extraordinary geometrical tunability, which opens new paths to obtain strong FR modes in the visible spectrum.

In this research article, we investigated individual, and periodic arrays of antisymmetric dimer structure composed of silicon concentric split nanoring resonators (SCRRDs) that are placed in a close vicinity of each other. To this end, we employed silicon NPs with the experimentally measured Palik constants [21]. Spectral response calculations of the individual split concentric ring resonator dimer (SCRRD) revealed multiple pronounced FRs in the visible spectrum. Polarization-dependence is the major advantage of the SCRRD which can be exploited in designing MM structures for switching applications. We also formed an all-dielectric MM by arranging the SCRRDs in a periodic fashion in both x and y directions on a quartz substrate as a meta-surface and numerically studied its optical characteristics. More specifically, we calculated the transmission spectra in different ambient conditions and investigated how the FRs shift with the ambient refractive index alterations. Sensitivity of the proposed MM to the ambient refractive index perturbations was quantified by calculating the FOM and FR shift over the refractive index unit perturbations (nm/RIU).

2. Theory and simulation

We used discrete dipole approximation (DDA) method and finite-difference time domain (FDTD) model (Lumerical FDTD Solutions software package 2015) for the theoretical and numerical analysis of the proposed structures. Details of the FDTD numerical analysis are as follows: the spatial cell sizes are set to \( d_x = d_y = d_z = 1 \text{ Å} \), with 250 000 numbers of cells, and perfectly matched layers as the boundary condition with 64 layers. In addition, considering numerical stability for the employed subwavelength components, simulation time step is set to 0.03 fs according to the Courant stability condition [22]. Both the SCRRD and MM are illuminated using a linear plane wave with a transverse electric polarization and the amplitude of 1.5854e-20 and pulse length of 2.6533 fs.

The proposed silicon dimers in an antisymmetric molecular orientation provide dramatic structural tunability which yields adjustability of the optical response with high accuracy. It is shown that the coupled electric and magnetic dipoles in a certain NP and also in a symmetric cluster consisting of a certain number of dielectric NPs can be characterized by using the DDA method, which includes periodic Green’s functions for both of the transverse and longitudinal polarizations [23, 24]. Using DDA and applying the effect of symmetry-breaking, the induced electric and magnetic dipole moments as a function of polarizability and dyadic Green’s functions are given by [24]:

\[
d^{p,m} = \alpha^{p,m} \left( F_{E,H} + \sum_{ij} \hat{G}_{ij}^{p,m} d^{p,m} \right)
\]

in which \( \alpha^{p,m} \) corresponds to the electric and magnetic polarizabilities of head-to-head silicon NPs, \( F_{E,H} \) are the exciting electric and magnetic fields in the certain area of the finite nanocluster or on a certain particle, and finally, for the interaction between proximal NPs, periodic Green’s functions are utilized (denoted by \( \hat{G}_{ij}^{p,m} \)). Moreover, polarizability has been employed to specify scattered electromagnetic (EM) field of particles in a periodic array or system [10].

3. Results and discussion

Figure 1(a) shows two schematic diagrams of the proposed molecular SCRRD, where two sets of concentric nanorings are located a few nanometers away from each other (the offset gap distance: ‘\( D' \)’) to provide desired coupling between the excited resonant modes. The geometrical parameters are introduced in the picture and their numerical values are given in the figure caption. It should be pointed out that the several variable structural parameters provide the mean to induce, control, and shift (blue/red) the position of FR modes over the bandwidth in the scattering cross-sectional profile. The investigated structure also yields strong polarization-dependency due to the geometry of the utilized split ring resonators. In this regime, split section angles in nanorings (\( \theta_e, \theta_m \)) satisfy the required antisymmetry condition to excite new magnetic dark modes in the dimer under linear plane wave illumination, where these split sections generate high order of electric and magnetic modes (multipoles). To characterize the EM-field excitation and formation of dipolar and multipolar EM-modes, we plotted the scattering cross-sectional profiles for an isolated silicon nanoring resonator as a function of incident wavelength for different split angle (\( \theta \)) values (see figures 1(b) and (c)). In these profiles, the spectral responses
for the inner and outer shells are depicted individually to show the effect of size of NPs as well. For instance, for the bigger shell with default geometrical sizes, for a complete circle ($\theta = 0^\circ$), a magnetic dipole peak is observed, and by increasing the size of split angle, a quadrupolar peak appears due to symmetry cancellation in the ring structure. In this regime, increasing the size of split angle led to a dramatic reduction in the amplitude of both magnetic peaks. Besides, the inner nanoshell shows almost the same behavior for the split angle varies with different scattering intensity. To show the effect of geometrical parameters on the scattering profile of a Si nanoring, we plotted the result of these modifications in figures 1(d) and (e). Noticing in figure 1(d), increasing the size of $c$ and $d$ to 355 nm and 450 nm and setting the split angle to $45^\circ$, a distinct magnetic dipolar peak ($P_D$) and two shoulders appear for quadrupolar ($P_Q$) and octupolar ($P_O$) resonant modes. For the smaller split ring, two distinct peaks are observed corresponding to the magnetic dipolar and quadrupolar peaks (see figure 1(e)). Then, we used both investigated split rings to design our proposed concentric ring resonator structure and eventually a simple dimer. Figure 2(a) exhibits numerically calculated spectral response for an isolated Si-SCRR under the illumination of a polarized linear plane wave in transverse direction. Obviously, the proposed silicon-based structure is able to support strong electric and magnetic resonant modes with a Fano-like dip in between (at $\lambda = 0.680 \, \mu m$). In this regime, by inducing the magnetic dipolar mode inside the SCRR, the electric dipolar peaks appeared at the split sections and outer part of NPs. Then, a destructive interference of magnetic and electric dipolar resonant modes led to the formation of this Fano-like resonant mode. Due to the limited energy of dipolar energy modes in a single SCRR unit, hence strong and pronounced Fano dip has not been observed. Furthermore, it should be noted that the quadrupolar modes do not have enough energy to couple effectively and induce a dip in the scattering response. In continue, with the placement of a couple of equivalent SCRRs and designing a Si-SCRRD, we would be able to intensify the energy of dipolar peaks to intensify the energy of FR mode. Also, because of having required energy, we expected a destructive interference between magnetic and electric multipolar modes that can be ensued by formation of an additional or second Fano dip. In terms of optical physics, in the near-field coupling regime and when two silicon-based structures become near each other with a few nanometer offset gap distance, arisen dipolar and multipolar magnetic modes couple to produce a narrow coupled magnetic response inside the NP structures. On the other hand, dipolar and multipolar electric modes couple to induce a wide electric response with an intense localization in the offset gap distance between NP structures. The result of this EM-field excitation and interference between the broad bright mode with the narrow and sharp dark mode in the Far-field is formation a FR dip in the scattering profile. This mechanism can be used to describe the formation of pronounced and multiple FR dips in more complex structures such as silicon-based a dimer (SCRRD). The small gap distance in a homogenous SCRRD yields a significant intensification in the excited magnetic and

Figure 1. (a) Three and two-dimensional schematic diagrams for the SCRRD with the descriptions of the geometrical parameters. (b), (c) scattering spectra for an isolated silicon nanoring for different split angle values for the inner (smaller) and outer (bigger) nanorings, (d), (e) scattering cross-sectional profiles for both inner and outer silicon nanorings for different geometrical parameters.
electric resonant modes. This intensification and enhancement in the local field causes to formation of deeper and narrower FR modes. Figure 2(b) illustrates numerically calculated scattering cross-sectional profile for the silicon dimer under transverse polarization excitation, where a linear plane wave is used as a light source with the spectral range of $\lambda=0.4-1.2 \, \mu m$. Noticing in the diagram, two distinct dips correlated with the FR modes at $\lambda=0.440 \, \mu m$, and $0.630 \, \mu m$ are excited. This figure also compares the achieved numerical results with the theoretical outcomes and a small difference between these diagrams is the appeared small dip in the theoretical analysis correlating with the accuracy between numerical analysis and theoretical computations. Therefore, to provide an exact research article, we utilized the numerical results in further analysis. It should be underlined that the effect of the edge to edge offset distance ($D$) is not significant in the silicon-based configurations [5, 6, 10], while it is extremely important in entirely metallic NP-based plasmonic structures. To prove this claim, we depicted the scattering cross-section profile for a SCRRD as a function of incident spectrum for six different offset gap distances ($D$) between proximal NPs (see figure 2(c)). Decreasing the size of the gap distance to 10 nm provides just a few nanometer red-shift of Fano dips and more decrements in this parameter cause to blue-shift in the position of FR modes which also includes a decadence in the narrowness and quality of FR dips. This destructive influence originates from the destructive overlap cancellation between dark and bright modes in the energy band of the bright mode. On the other hand, increasing the size of gap distance leads to losing the Fano dips due to disappearing of magnetic and electric multipolar interferences. Also, at large distances, the multipolar modes do not have enough energy to interact with dipolar and multipolar modes of the adjacent nanostructure. As a result, we observe a significant blue-shift in the position of shallow and broad dips. Herein, to provide a structure with easy fabrication, we set the gap distance to 15 nm which shows a reliable optical response in numerical and theoretical studies. Figure 3(a) illustrates two-dimensional snapshots for the electric $|E|$ and magnetic $|H|$ field excitation and coupling between proximal NP arrangements with a demonstration of modes between interior and exterior split nanorings. The magnetic dipole moment in the interior and exterior nanorings can be in or out of phase for different incoming wavelengths and polarizations. Thus, the induced magnetic dipole moments oscillate in opposite directions in a concentric system of silicon nanorings. In order to clarify the role of opposite modes inside a SCRRD, we plotted the charge distribution direction inside the examined all-dielectric dimer system in figure 3(b), wherein the opposite direction of current distribution in the exterior and interior nanorings verifies the hypothesis that is proposed by the correlated theoretical, analytical, and experimental publications [10, 23, 24]. Figure 3(a) shows a three dimensional schematic diagram for the proposed MM, where silicon SCRRDs are deposited on a quartz substrate, periodically. The distance between two neighbor dimers for
both x and y-axes is set to 100 nm, where the overall size of the proposed MM is exactly 6.2 × 4.5 × 1.1 μm. Considering each one of SCRRD unit cells as a meta-atom, and depositing them on a SiO2 substrate as a meta-surface with the thickness of \( h = 1 \) μm and with the relative permittivity of \( \varepsilon = 4.5 \), we tailored an all-dielectric MM structure to support strong FR dips in the visible spectrum. The thickness of SCRRD units was set to 85 nm. The height of the structure with the quartz substrate was selected based on calculated absorption coefficient and the effect of the substrate on the amplitude transmission profile. In this regard, Campione et al [25] and Ahmadivand et al [26] have examined the effect of dielectric meta-surface on the absorption coefficient of the propagating optical power by determining the electric and magnetic polarizabilities of the NPs in oligomer clusters in molecular levels, where periodic Dyadic Green’s functions and polarization angle plays a fundamental role in this series of theoretical computations. Illuminating the all-dielectric MM by a transverse polarization (\( \alpha = 0^\circ \)), the amplitude transmission spectrum was calculated numerically (see figure 4(b)), and two strong and deep FR modes were found around \( \lambda \sim 0.443 \) μm and 0.655 μm. Figure 4(b) also compares the transmission amplitude for the MM for the variations in the polarization angle. As obvious it is, changing the polarization angle of the incidence beam (\( \alpha \)) in the range of \( 0^\circ < \alpha < 30^\circ \) gives rise to dramatic decadence in the quality of both of the Fano dips, where for \( \alpha < 30^\circ \), FR dips disappear totally. Hence, the polarization-dependency of the presented MM is verified numerically with a high accuracy. Figure 4(c) illustrates the magnetic field propagation and transmission along the all-dielectric MM structure by a two-dimensional snapshot. In this snapshot, the energy of the magnetic field at the NP dimers is obvious. The low-loss nature, narrow and deep FR dips, and polarization-dependency of the investigated MM would allow high accuracy sensing applications.

The accuracy of an all-dielectric MM sensor can be defined by determining the sensitivity (S) and quantifying corresponding FOM. To evaluate the quality of the proposed all-dielectric MM, we examined its optical response to the refractive index perturbations in the surrounding medium. Hao et al [27] and Anker et al [28] have recommended a practical method to define the sensitivity of plasmonic biosensors based on the behavior of the appeared resonant modes to the variations in the refractive index of the environment. For dielectric nanostructures the same mechanism is applicable. We used various liquid-type substances with different refractive indices to evaluate the behavior of the appeared FR dips in the amplitude transmission spectra. Illuminating the structure with a transverse polarization, and immersing the structure in the following liquids: Fluorine refrigerant R-22 with \( n = 1.26 \), Silicon oil with \( n = 1.33 \), 60% Glucose solution in water with \( n = 1.43 \), Chlorobenzene with \( n = 1.52 \), and Aniline with \( n = 1.58 \), we calculated the amplitude transmission spectra as depicted in figure 5(a). Clearly, increasing the refractive index of the surrounding medium gives rise to distinct red-shifts in the position of both of the FR dips and Fano minima become sharper and narrower. Plotted diagram as an inset in figure 5(a) exhibits the shift of Fano dip for the free space and a liquid with the refractive index of \( n = 1.26 \) as a surrounding medium that was calculated as \( \Delta \lambda = 4.19 \) nm. To determine the sensitivity of the structure, we plotted a linear fit (see figure 5(b)) for the FR modes positions over the refractive index changes, where the slope of the line defines the sensitivity for the MM which was found to be 497 nm/RIU. Using the widely accepted relation for FOM: FOM = \( S/\Delta \lambda \) [27, 28], for \( \Delta \lambda = 4.19 \) nm, we calculated that FOM = 118.5 for the proposed MMMs. A comparison of both obtained sensitivity and FOM for the studied MM with the other all-dielectric MMMs in the literature reveals the superior behavior of the current structure [26]. Figure 6 exhibits the effective permittivity spectra for both real and imaginary parts used to determine the surface sensitivity of the MM. The inset shows the reflection spectrum for the all-dielectric MM where reflectance at the sharp Fano dips appear to be negligible. These diagrams could be used to prove the preciseness and

![Figure 3.](https://example.com/f3.png) (a) Two-dimensional snapshots of the electric \(|\mathbf{E}|\) and magnetic fields \(\mathbf{H}\) excitation inside the SCRRD and between concentric split nanorings, (b) charge distribution direction inside the dimer system that proves the interference between dark and bright modes to generate FR dips. 

}\[\text{RIU} \text{. Using the widely accepted relation for FOM: FOM} = \frac{S}{\Delta \lambda} [27, 28], \text{for} \Delta \lambda = 4.19 \text{ nm}, \text{we calculated that FOM} = 118.5 \text{ for the proposed MMMs. A comparison of both obtained sensitivity and FOM for the studied MM with the other all-dielectric MMMs in the literature reveals the superior behavior of the current structure [26]. Figure 6 exhibits the effective permittivity spectra for both real and imaginary parts used to determine the surface sensitivity of the MM. The inset shows the reflection spectrum for the all-dielectric MM where reflectance at the sharp Fano dips appear to be negligible. These diagrams could be used to prove the preciseness and...}
sensitivity of the proposed MM based on the method introduced by Yeatman et al [29]. For the studied MM with the effective permittivity of \(\varepsilon_{\text{eff}} = \varepsilon' + \varepsilon''\) in the air ambience (\(\varepsilon_0\)), the reflection (R) curve slope is given by \(\frac{dR}{dk_z}\), where \(k_z\) is the wavevector of the propagation direction. The sensitivity can be determined by [29]:

\[
\frac{dR}{dk_z} \approx \frac{3\sqrt{3}}{2} \frac{\Gamma'\Gamma''}{(\Gamma' + \Gamma'')^3},
\]

where \(\Gamma'\) is the intrinsic loss factor, and \(\Gamma''\) is the re-radiative loss term. It is well-accepted that for sharp resonant dips, the reflection is close to zero \(R \to 0\), hence, we have \(\Gamma' = \Gamma''\) [26, 30]. Finally, to detect any perturbation in the surrounding refractive index, we used the sensitivity limit, which is resulted from the slope at the enhanced coupling regime:

\[
dk_z = \frac{9N}{4\sqrt{3}N_0^3 k_0 \varepsilon''},
\]

where \(k_0\) and \(n_0\) are the wavevector and refractive index of the incident beam in the ambient, respectively, and \(N\) is the noise to signal ratio. For an incoming light with an intensity of 1 mW, and \(N \sim 0.001\), we can rewrite the formula above as a function of refractive index variation giving the minimum sensible variation in the ambient refractive index as [29]:

\[
dn_0 = \frac{1.3Nn_0^3\varepsilon''}{\varepsilon'^2}.
\]

By considering the effective permittivity of the proposed all-dielectric structure, for instance, at the FR mode position (\(\lambda \sim 0.655\, \mu m\)) for the air and Aniline (liquid) environments the sensitivity can be found as \(38 \times 10^{-5}\) and \(61 \times 10^{-5}\), respectively. Considering all of the achieved data for our structure, the proposed all-dielectric MM with the deposited SCRRDs has comparable sensitivity with various plasmonic structures [31, 32] with the additional advantage of low-cost and easy fabrication. Besides sensing applications, using its polarization-dependency, the proposed MM has a strong potential to be used as a router for optical modulation such as Fanoswitches.

4. Conclusions

In this work, we investigated the spectral response and optical features of an all-dielectric MM structure with the deposition
of silicon SCRRD nanostructures as meta-atoms on a SiO$_2$ substrate. We showed that the proposed structure can be tailored to support multiple strong FR modes in the visible spectrum. Using numerical and analytical methods, we calculated the amplitude transmission spectra of the structure for different refractive indices of the surrounding medium. We also demonstrated the polarization-dependency of the proposed all-dielectric MM. The sensitivity and FOM as of the investigated MM were calculated as 497 nm/RIU and 118.5, respectively. This work opens up avenues for developing easy to fabricate, low-cost, polarization-dependent, and high-precision biochemical sensing devices, as well as fast routers and Fano switches in nanoscale.

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