



Nanoparticle using parallel split rings and implementation of chain for creating Fano resonance with polarization independence for energy harvesting in mid-infrared

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Abstract

In optical devices, the polarization of the incident wave affects the Nano particle characteristics. Therefore, designing a polarization-independent device is significant in the process of designing optical structures. On the other hand, the concept of Fano resonance and dark mode has been utilized for achieving more energy enhancement. In this paper, we have developed a symmetrical Nano antenna by employing Fano resonance, which is independent of the incident wave polarization. The proposed Nano antenna is modified in mid infrared regime for biosensing and energy harvesting applications. The designed metamaterial antenna is made by Nano split ring resonators with etched capacitive gaps, which are utilized for concentrating energy. The introduced Nano antenna has a bright and dark mode with a weak enhancement of electric field. The effect of the incident wave polarization is investigated at wave incident angles between 0° and 45° to illustrate the independency of the polarization due to the symmetrical shape of the Nano antenna. In order to trigger the dark mode and enhance the electric field, a Nano chain is incorporated in the final structure. This arrangement has led to increasing of electric field drastically. Furthermore, the figure of merit has been calculated as an advantageous factor in sensing the surrounding materials with various refractive indices. Our findings illustrated that the chain arrangement has caused a peak in the linear form of the extinction cross section of the Nano antenna. This in turn has resulted in the appearance of Fano resonance with no impact on the resonance frequency that has been originally adjusted by capacitive gaps and inductive strips.

Keywords FANO resonance · Controllable field enhancement · Plasmonic · Dark mode

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1 Introduction

Surface plasmons are the key elements in the optical science and properties of these critical elements has been analyzed and exploited for numerous technological applications. Plasmons are associated with oscillations of surface electron density on metal–dielectric interfaces (Nouri-Novin et al. 2018; Bazgir et al. 2018), and plasmonics is the study of the interaction between electromagnetic fields and free electrons in metal in the way that free electrons can be excited by the electric component of light to have collective oscillations (Xu et al. 2016; Sadatgol et al. 2015). Recent advances in nano-fabrication, characterization, and modeling techniques have allowed unique properties of these surface electromagnetic modes to be explored with respect to subwavelength field localization and wave-guiding, opening the path to the realization of a truly nanoscale plasmonic optical absorber (Wang et al. 2017). This area of investigation also has interesting links to research on photonic band gap materials and the field of optical metamaterials (Kelf et al. 2005; Rufangura and Sabah 2016). Nowadays, Plasmonics has become the interdisciplinary area of many types of research which attracts scientists' attention from different backgrounds such as chemistry, physics, optics, and engineering in order to discover and exploit new applications and properties of surface plasmons (Keyser 2016; Giner-Casares and Liz-Marzán 2014). Current and forthcoming discoveries have impacts in various fields of science and technology, including photonics and material science, biology and medicine (Nouri-Novin et al. 2019; Austin et al. 2015).

Fano resonances, on the other hand, have been noticed for their attractive attributes in optical research, such as asymmetric line-shape, sharp spectral features, and sensitivity to structural and electric field enhancement. The interaction between non-radiative (dark or quadruple) modes with radiative (bright or dipole) modes causes the asymmetric line shape of the resonance (Chong et al. 2014). Dark mode is the concentrative localized mode which leads to higher energy enhancement in a limited area of nano-antenna. On the other hand, the bright mode exhibiting radiation characteristics covers a larger area of the antenna with a lower state of energy (Verellen et al. 2011; Wang et al. 2015). During the last decade, various shapes of nano-antenna (Rahmani et al. 2013) and nano-cluster (Fan et al. 2010) have been studied to achieve Fano resonances which can be categorized in two main groups of asymmetric and symmetric nanoparticles (Panaro et al. 2015; Farmani et al. 2018). Various shapes of the nanocluster in symmetrical formation for the Fano resonance such as gold nano-disks clusters (Chong et al. 2014), second harmonic generation by plasmonic heptamers (Thyagarajan et al. 2013), and plasmonic aluminum nano-particle clusters (Ahmadivand et al. 2015) have been developed. On the contrary, Nano antennas with asymmetric formation are more applicable in arousing the Fano resonances of structures, including the ring/disk plasmonic Nano-cavities (Cetin and Altug 2012), plasmonic nanostructures and metamaterials (Lukyanchuk et al. 2010) and also for inductive tuning of Fano-resonant metasurfaces with graphene (Mousavi et al. 2013).

The metamaterial shapes have also been explored in the optical regime for plasmonic multi-resonance applications in biosensing (Turkmen et al. 2011; Cetin et al. 2012). Moreover, various models of them have been designed to create Fano resonances (Çetin et al. 2011; Wu et al. 2012). Second harmonic generation for the optical and the infrared regime is also made for obtaining multi Fano resonances (Shadrivov et al. 2006). Split ring resonators (SRRs) are the most common designs for diverse applications in various shapes and arrangements where gaps are important in controlling the resonance (Lahiri et al. 2013; Xu et al. 2014).

However, the symmetrical structures are desirable to have independency to the polarization of the incident wave (Farmani et al. 2018) and are studied to create the second harmonic generation for higher energy enhancement (Liu et al. 2016).

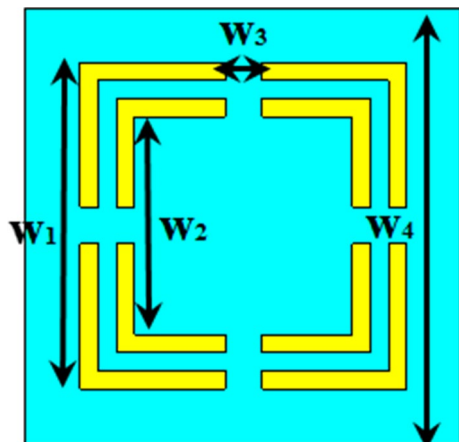
In the present work, we developed a symmetrical SRR cluster to achieve Fano resonance, which is independent of the incident wave polarization at mid-infrared applications for bio sensing. The figure of merit (FOM) Heydari et al. (2017) is calculated for four various materials and the shift of resonance wavelength are also obtained from the curve of the extinction cross section. At first, we developed a nano-antenna based on SRR structure. However, this structure shows two bright mode resonances, therefore in the second step, the chain is added and the dark and bright modes are observed. Using this method, we have succeeded to increase the electric field enhancement drastically.

2 Nano particle design and simulation setup

Figure 1 shows the top view of the proposed Nano-antennas which is studied for achieving Fano resonance. The special SRR cluster with the total size of the $900 \times 900 \text{ nm}^2$, and the width and thickness of 50 nm and 40 nm, respectively, are used as the nano-particle. The inner and outer rectangular rings are separated by a gap of 50 nm.

The nano-structures are designed over the 50 nm thick SiN substrate with refractive index of 1.98 and the total dimension of $1200 \times 1200 \text{ nm}^2$. The incident plane wave with the intensity of 1 V/m polarized along the X direction is emitted normally to the cluster. To study the optical properties of the proposed parallel split rings, we have used the Mie scattering theory and time domain FIT method for the numerical simulation. In addition, for designing and simulating the proposed parallel SRRs and the implemented chain, we have employed a commercial software package CST Microwave Studio, and used the 'open' boundary conditions for our simulation environment while the hexahedral mesh formation is utilized with the reflection level of around 0.001 at the boundary. The Palik model is chosen for the material modeling of gold at the optical regime and negative permittivity in the optical domain based on Drude model. Moreover, all the mentioned parameters in Fig. 1 are as $W_1 = 900 \text{ nm}$, $W_2 = 700 \text{ nm}$, $W_3 = 100 \text{ nm}$, and $W_4 = 1200 \text{ nm}$.

Fig. 1 The top view of the proposed Nano-antennas and the geometry of the nano particle

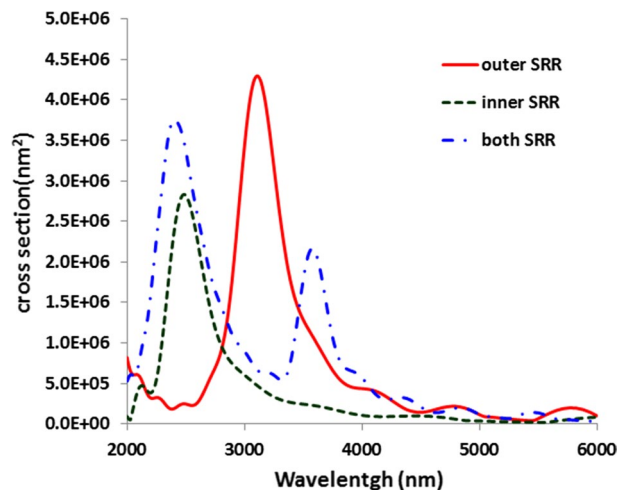


3 Simulation result

For specifying the Fano resonance, the curve of the extinction cross section (ECS) is obtained and investigated. ECS is important in bio-sensing applications and obtaining the FOM factor for surface enhanced Raman spectroscopy (SERS) (Zarrabi et al. 2016). For achieving Fano resonance, the interaction between two modes is necessary, so we proposed to implement two rings having a coupling with each other. Figure 2 shows the ECS for each ring separately and also for the coupled structure. As can be seen in Fig. 2 both inner and outer rings show single resonances at $\lambda_1=2500$ nm and $\lambda_2=3100$ nm respectively. However, the proposed nano-antenna has two resonances at $\lambda_1=2400$ nm and $\lambda_2=3500$ nm and at these wavelengths, the maxima of the ECS are around $3.6E+06$ and $2.1E+06$ nm², respectively. Here, as shown in Fig. 2, we have a Lorentzian formation for single inner or outer SRR and the maximum value of the ECS is $4.5 E+06$ nm² for outer SRR. Besides, the ECS for inner SRR is less than the outer SRR and so we can come to this conclusion that the ECS is related to the size of the Nano-particle. Drop in the ECS spectra is originated from the alteration of modes of the structure since we have a bright mode for each SRR and when they couple we see one bright and one dark mode. The dark mode is a non-radiative mode, and we typically expect low cross section for the non radiative mode as shown in Fig. 2. The coupling and interaction between elements in Nano-antennas are also shown in Ahmadivand et al. (2016).

Figure 3a–d presents the electric field enhancement for the outer ring and inner ring separately and also the combination of them at their resonances. As shown here, the energy has been concentrated in the place of gaps, and the gold layers are responsible for creating an inductive property for each of resonances. When the inner and outer rings are coupled, a multi-resonance structure is created and by increasing the frequency (reducing the wavelength), the energy is concentrated mostly in inner ring gaps. In this structure, we can model the antenna with a simple LC equivalent circuit and frequencies of resonances can be calculated by $f_1 = 1/2\pi\sqrt{L_1C_1}$ and $f_2 = 1/2\pi\sqrt{L_2C_2}$, where the capacitors for both rings are inversely related to the gap and equal with each other, $C=C_2=C$. In addition, the inductance is related to the length of L-shaped element and

Fig. 2 The extinction cross section of coupled rings, single inner and outer ring



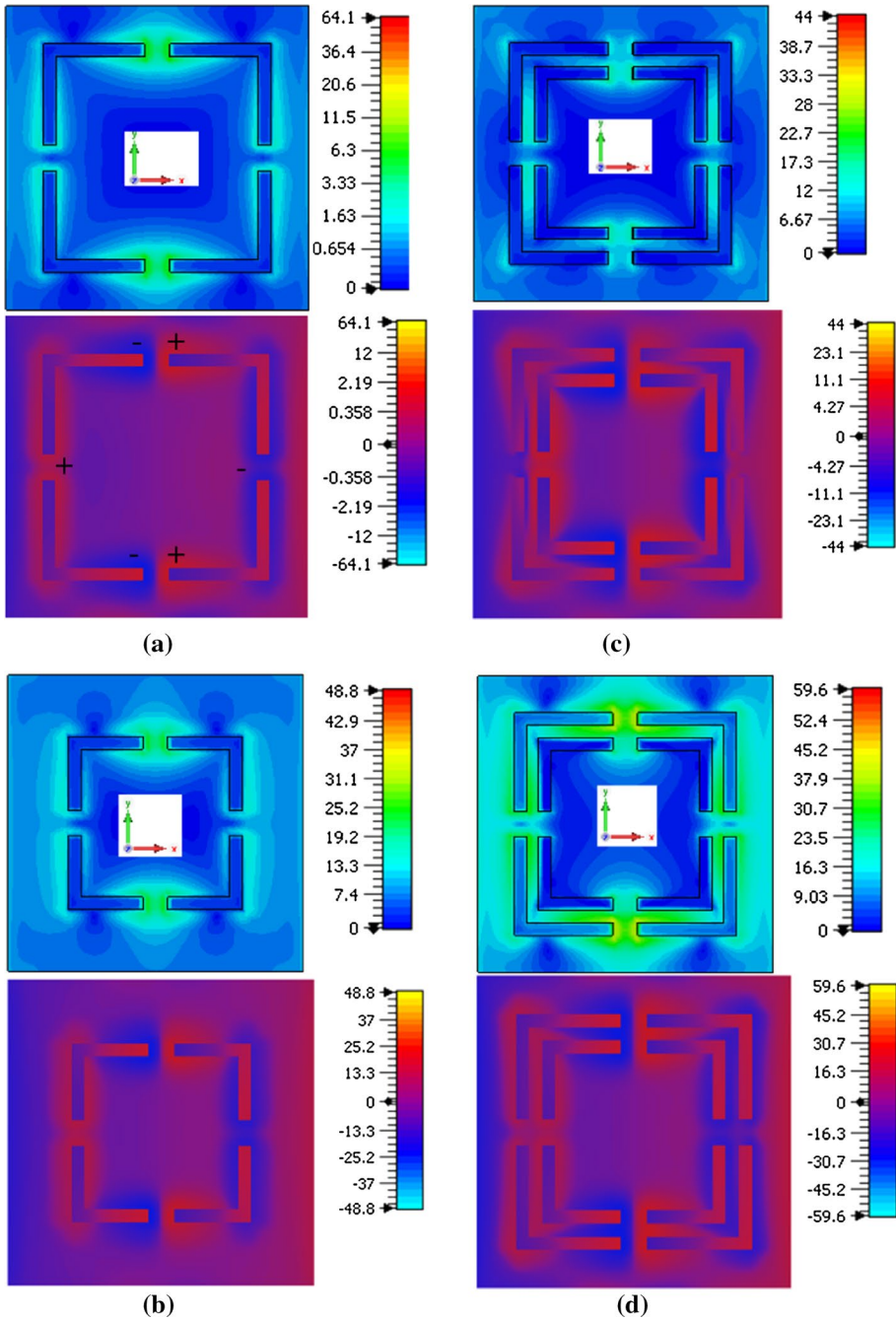


Fig. 3 Electric Field distribution for prototype Nano-antenna at **a** the simple outer ring at 3100 nm, **b** the simple inner ring at 2500 nm, **c** the coupled inner and outer rings at 2447 nm, and **d** the coupled inner and outer rings at 3600 nm

then $L_2 = 0.73L_1$. Therefore the resonant frequency changes inversely proportional to the square root of the ratio of the inductances.

Figure 3a, b show that the maximum fields are concentrated in the upper and lower gaps, which results in a dipole mode for these two cases, and the electric field dispensed in gaps and the metal edges while they distribute on the surface of the dielectric. In the final model when two ring structures are combined, we encounter a different state, as shown in Fig. 3c, the maximal field is gathered in the upper and lower gaps, indicating the dipole mode as well. However, at the next resonant frequency, the electric field is dispensed in dipole mode, but we should notice that in this case, field is between two SRRs and the field is increasing more than the first resonance. Therefore, we expect an increase in the intensity of the field, as shown in Fig. 3d. By extracting the ratio of energy intensity ($|E^2|/|E_{int}^2|$)

where E_{int} is incident field), we succeed to achieve 4096 times enhancement in the first structure and 2304 times in the second one. But in the structure coupled rings, this value is increased to 5536 times at the dark mode resonance which also shows the quadruple mode.

The results show that by increasing the size of SRR the electric field is also increased, which is due to more plasmon polariton at the interface of gold and dielectric.

Polarization independence in negative-index metamaterials (NIM) has been investigated for microwave and optical regime in various applications such as absorbers and nano-antennas (Aydin et al. 2008; Giloan and Astilean 2012). Recently, various models of polarization independent nanoantenna are examined utilizing Fano resonance and second harmonic generation (Liu et al. 2016; Zarrabi et al. 2017). The symmetrical structure is very attractive to create Fano resonance and therefore, in this study we have simulated different angles of polarization to investigate the dependency of the structure to polarization angle. To this end, we checked four polarization angles from 0° to 45° . The simulation results are presented at Fig. 4, which is confirming the idea that the proposed structure is independent of polarization angle.

In this structure, as mentioned in Fig. 3, the electric field is accumulated in the gaps while four gaps on the four sides improve the stability of the structure. Therefore, changes in the angle of incident wave are controlled by orthogonal gaps.

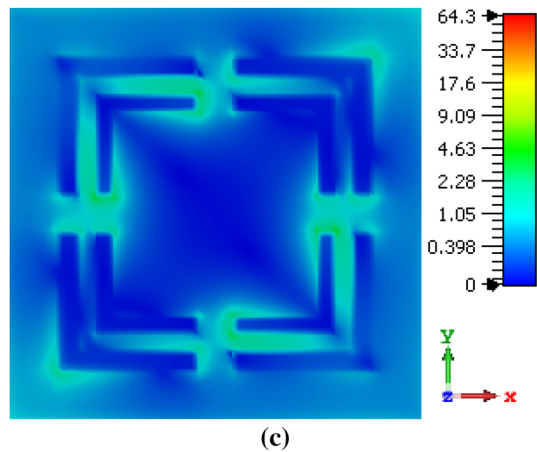
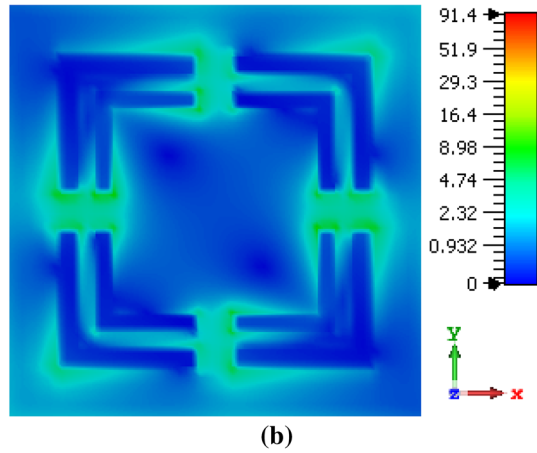
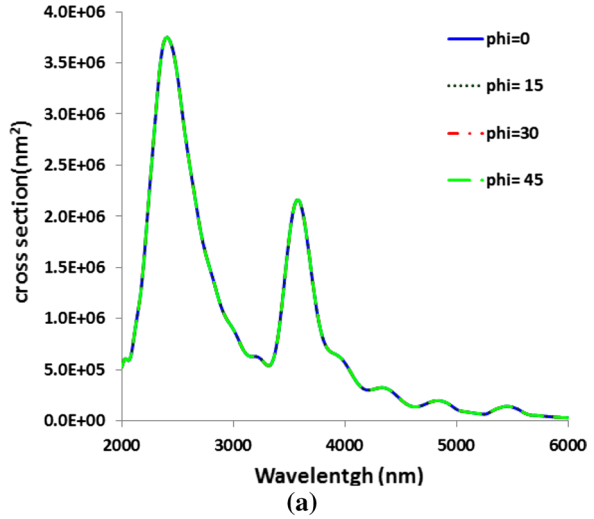
The overall size of the Nano antenna would be larger in the diagonal direction for various angles of polarization. Consequently, when the object has a symmetrical formation, it has less frequency shift or extinction cross section values as other elements compensate this distortion. In addition, the gaps can control the electric field but the larger effective length of the antenna will make more surface plasmon and as a result the gaps concentrate more energy (Fig. 4b, c).

The chain or nano-particle array in the straight line with various shapes of spherical, disk and rod has been developed for guiding the energy in the optical regime with various materials such as silver, gold and aluminum (Willingham and Link 2011; Ross and Schatz 2014). As Fig. 5a illustrates, the chain structure is implemented in a cross-shape at the center of symmetry of the SRR structure. The chain includes spherical particles and the radius of the sphere is selected 30 nm while the distance between centers of two spheres is chosen to be 83 nm. According to Bajestani et al. (2011) the distance between these two nanoparticles center should be typically between 2 and 3 times greater than the radius.

Nanoparticles absorb the scattered fields at the surface of the antenna and then fields are transmitted by the transmission lines created by the chain. In addition, the last nanoparticle is located between the gaps, which make them change and save more energy.

In the structure with chained nano-spheres, the incident wave (E_{int}) is assumed 1 V/m and we see that the dark mode scattered electric field (E_{sc}) is increased to 203 V/m

Fig. 4 **a** The extinction cross section for various polarization angles between 0° and 45° , **b** the electric field distribution for 45° at 3600 nm, **c** the electric field distribution for 45° at 2500 nm



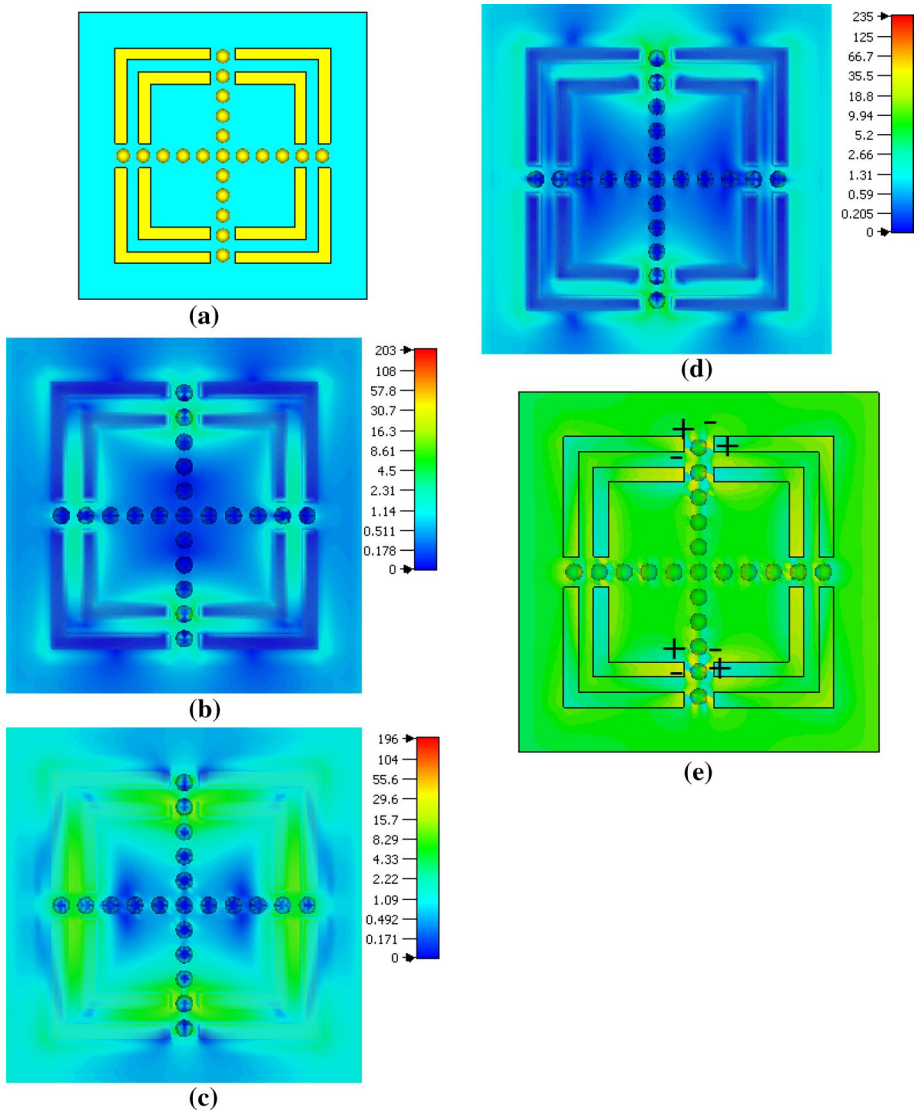


Fig. 5 **a** Implementation of the chain in nano antenna arousing the dark mode and Fano, **b** the field density for dark mode at 3600 nm, **c** the field density for bright mode at 2477 nm, **d** the field density for Fano dips, **e** the charge dispensing for Fano dips

(Fig. 5a) while at the first structure (without chain), it was around 59.6 V/m (Fig. 3c). The concentrated energy is calculated by (1) Sendur et al. (2011).

$$P = \iiint_{V_M} \sigma |E^2(r)| \cdot dV = \iint_S \left(\frac{1}{2} E(r) \times H(r) \right) \cdot \hat{n}_s ds \quad (1)$$

where ‘ σ ’ is the layer conductivity and ‘E’ and ‘H’ are electrical and magnetic fields, respectively, and $E(r) = E_{\text{int}} + E_{\text{sct}}$. Therefore, when the electric and magnetic field energy

increase, we suggest chain structure to improve the electric field in the surface of the antenna. As the results as shown in Fig. 5b, c, the electric field is enhanced by the proposed method and it has increased from 59.6 to 235 V/m at the second resonance at 3600 nm, and from 44 to 203 V/m at the first resonance at 2477 nm.

Hence, we have more than 393% enhancement by excitation of the dark mode and at the second resonance, this enhancement is around 460% where the electric field is around 203 V/m for the bright mode (dipole mode) (Fig. 5b). The Fano dip Verellen et al. (2011) is made between the bright and dark mode at 3189 nm where we have drastically increased the electric field around 196 V/m and the charge would be concentrated at this point with an unusual distribution, not similar to the dipole nor quadrupole formation (Fig. 5c). This point is very noteworthy because for the proposed antenna without chain, we do not see Fano mode between two bright modes.

In brief, the gaps between SRRs (see W_3 at Fig. 1) are the main source of capacitances, and the chains are harvesting the dispensed electric field and conduct them to these gaps. Therefore, the electric field is extremely intensified in comparison to the basic model at Fig. 3d.

In Fig. 6, we have shown the extinction cross section for the nano-antenna in the presence and absence of the chain. Also it is shown that, the chain made a very negligible effect on the cross section, it could cause a notable effect on the field distribution.

To investigate the viability of using these structures in bio-sensing applications, we have selected four various prototyped biomaterials as in our previous researches with the thickness of 80 nm, where they were placed over the substrate and have surrounded our proposed Nano-antenna. The above mentioned materials under investigation are Ether (R–O–R') with $n = 1.35$, Ethylene glycol (HO–CH₂CH₂–OH) with $n = 1.43$, Chlorobenzene (C₆H₅C₁) with $n = 1.525$, and Quinoline (C₆H₇N) with $n = 1.627$ (Heydari et al. 2017). The frequency shifts in the extinction cross section are compared in Fig. 7a, b for the proposed antenna with (first antenna) and without chain (second antenna), respectively. As illustrated in this figure, the cross section is shifted to higher wavelengths by increasing the refractive index of the surrounding material. By comparing Figs. 6 and 7, we see for the first antenna that the wavelength at the first resonance shifts from 2404 to 2608 nm. For the second antenna, the resonance shifts from 2459 to 2702 nm which shows seemingly a higher frequency shift with respect to the structure without chain. The second resonance is also shifted for the first antenna from 3571 to 3973 nm, and for the second antenna from 3592

Fig. 6 The extinction cross section of nano antenna with and without chain

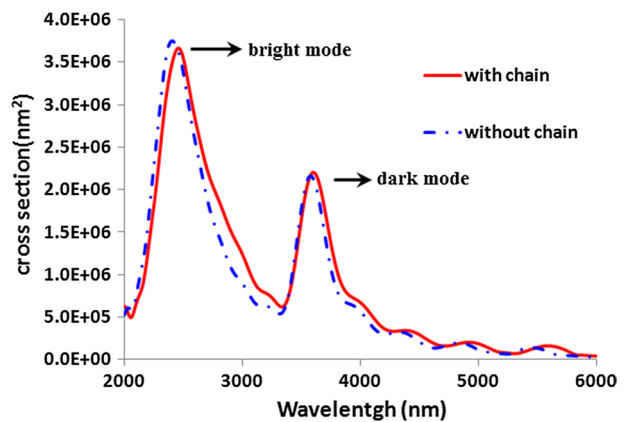
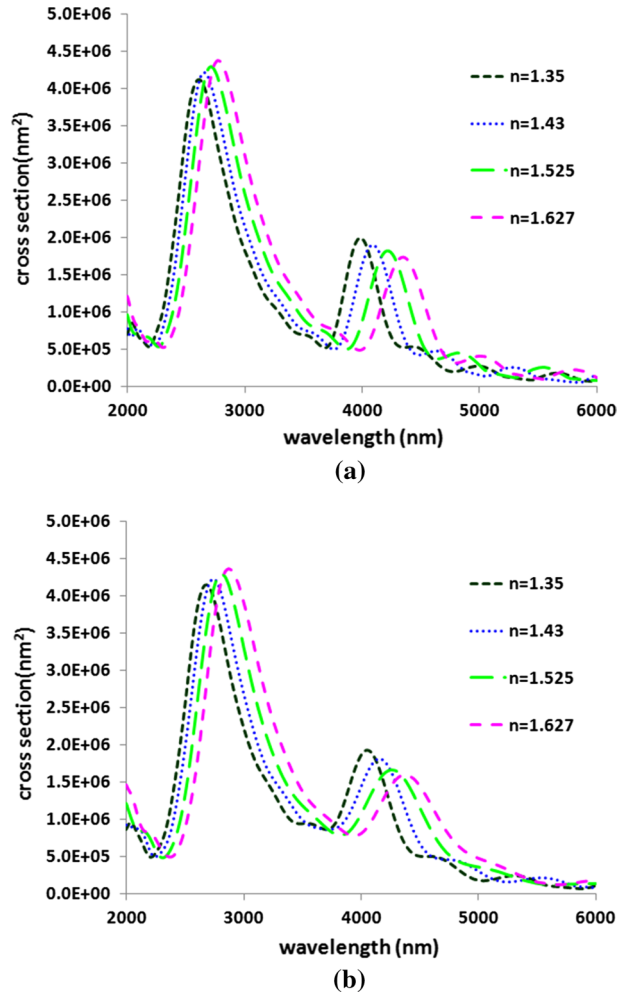


Fig. 7 The extinction cross section for various materials **a** for prototype metamaterial antenna without chain, **b** for prototype metamaterial antenna with chain



to 4054 nm, which is again an improvement over the first structure. All the above improvements denote that FOM factor in the nanoantenna with chain is more than that in the first antenna without chain. The material refractive index variation affected the extinction cross section at bright and dark modes, but as shown in Fig. 7 it has no effect on Fano dip resonance extinction cross section.

For fabrication of the mentioned metamaterial structure, split ring resonators (SRRs) based on plasmonic characteristic is used by performing electron-beam lithography micro-Fourier-transform infrared spectrometer equipped with an infrared microscope. Then thin layers of gold on the SiN layer were deposited uniformly by electron-gun evaporation, and finally the redundant resist was lifted off (Chen et al. 2008). The chain layer can also be deposited separately inside the metamaterial SRR (Barrow et al. 2011).

The wavelength shift is a parameter for defining the FOM of a sensor. The FOM is obtained by (2) and the results are presented in Tables 1 and 2 for both resonances:

$$FOM_t = \frac{\Delta\lambda}{\Delta n} \quad (2)$$

Table 1 The FOM of both structures for various materials for first resonance

	n = 1.35	n = 1.43	n = 1.525	n = 1.627
First structure	457.1429	479.0697674	483.8095	503.9872
Second structure	770.204	769.0697674	776.9524	736.5231

Table 2 The FOM of both structures for various materials for the second resonance

	n = 1.35	n = 1.43	n = 1.525	n = 1.627
First structure	1087.171	1136.355007	1204.48	1203.869
Second structure	1378.776	1384.119601	1302.612	1288.79

Table 3 The FOM comparison between current work and previous research

	FOM	Wavelength (nm)	Antenna structure
This work	1378	4000	Nanoparticle
Nouri-Novin et al. (2019)	228	1870	Nanoparticle
Heydari et al. (2017)	1031	4200	Nano aperture
Heydari et al. (2017)	2370	3200	Nano aperture

As shown in both tables, by implementation of the chain structure the FOM value is increased.

Typically various kinds of the nanoantenna have been utilized for bio sensing and the aperture or nanoparticle antennas have been considered for this goal. The comparison of the current work and previous models is presented in Table 3.

4 Conclusion

In this paper, the interaction of Subwavelength particles in chain formation with Nano-antenna has been studied. The proposed antenna without chain has created two bright modes with lower electric field enhancement, and when the chains of nano-spheres are implemented, one of the bright modes has changed to dark mode. Moreover, the electric field is enhanced drastically in both resonance and interaction between dark and bright has made a Fano dip. The FOM factor has been compared for both structures at various external materials, and we showed that the chain has noticeably improved the frequency shift. Here, we succeeded to show that the Fano dip is useful for bio sensing while the material has made the linear shift in the frequency of Fano dips.

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