Design and parametric simulation of triangle nano-particle structures for the visible and near-infrared frequencies

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Abstract

In this paper, the cross bow-tie nano-antenna (CBNA) with dimensions around wavelength of incident light is designed and simulated, with an emphasis on absorption cross section, absorption and reflection coefficients, as well as the electric field enhancement, in the visible and near-infrared spectral regime. The optical properties of the proposed nano-antenna have been investigated in details based on its geometric parameters and material type (for patch, substrate and the medium surrounding the antenna). Then the array of unit cell of proposed CBNA has been performed. The spectral response of the nano-antenna can be adjusted by geometric parameters, which provides control over the spatial resonance position and electric field enhancement amplitude. The CBNA with due to symmetric shape along the antenna's length and width, is less sensitive to incident light polarization. Since the polarization of incident light is not selective and this nano-structure can enhance the incident light in both directions x and y, so it will be useful for optical energy harvesting. In order to determine the resonance properties of CBNA, computer simulation technology (CST) microwave studio (© 1998–2018 CST), as a three-dimensional electromagnetic field solver based on finite integration technique (FIT), is used for simulations. Commercial software, FDTD (finite difference time domain) Solutions (© 2013–2017 Lumerical Inc.), available from Lumerical corporation, is also used to calculate the amount of absorption, reflection and transmission coefficients of the CBNA.

Keywords Optical nano-antenna · Bow-tie nano-antenna · Resonance · Surface plasmon · The visible and near-infrared spectrum

1 Introduction

Antennas are important in microwave and radio frequency regime because of their ability to efficiently transmit or receive electromagnetic energy between a local source and free-radiation fields [1]. The characteristic dimensions of an antenna are the order of magnitude of its radiation wavelength, and so the length of an optical antenna is limited to only a few hundreds of nano-meters. Fortunately, at present, the design and characterization of metal structures in nanoscale with a fabrication accuracy of ± 5 nm is achievable due to the development of nanotechnology. Nowadays, some standard techniques such as electron beam

lithography (EBL) are able to provide high resolution and control of pattern design, so they will be useful for fabrication of nano-structured planar samples. The light with a wavelength of about one micrometer cannot be stored or guided in dimensions smaller than half its wavelength. Hence, the diffraction limit is a fundamental limitation in optical frequencies. Plasmonic, as a new branch of photonics, is a good candidate to reduce the dimensions of the optical beam from three dimensions to two dimensions, overcoming the diffraction limit of light and concentrating light. Plasmonic is a resonance phenomenon based on the interaction of light with conduction electrons in nano-structured metals [2]. The oscillating electromagnetic

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fields at optical frequencies can penetrate metal particles. Therefore, metals in optical frequencies are not perfect conductors. The depth of penetration is defined by the skin depth of the material, which is very relevant at the optical spectrum [3].

Surface plasmon polaritons (SPP) and localized surface plasmon (LSP) are two main components of plasmonic. When metal nano-structures contain a dielectric (with a positive real dielectric constant) and a metal (with a complex dielectric function that the imaginary part of it is positive and small, and real part of it is large and negative), are illuminated by light, at the interface of metal and dielectric, collective electron oscillations can be excited [4]. SPPs are surface excitations that can confine the incident light in the perpendicular direction at the interface at a sub-wavelength scale. SPPs are due to indirect interaction (through prism, grating and etc.) incident light (only with TM polarization) and metal nano-structures. The interaction of light with the curvature of the surface of metal nano-particles leads to the coupling of conduction electrons with the incident electromagnetic field. LSPs are non-propagating excitations due to the direct interaction of light with metal nano-particles, which are caused by a scattering phenomenon, and exist for both TE and TM (transverse electric and transverse magnetic) polarizations. The interacting amount of light with the nano-particle depends on the size, shape and composition of the nano-particle and environment of it [5–7].

The interaction of light with metal nano-structures due to the frequency dependence of the metal complex dielectric function [8, 9]. Resonances of nano-structures composed of noble metals with sub-wavelength dimensions, usually occur in the optical spectrum. The performance of the optical antennas in increasing and also confining the incident light to a small volume, in addition to the proper design of the geometric shape and the dimensions of the composition, depends on the properties of surface plasmon resonances. Optical antennas based on the plasmonic phenomenon by controlling of sub-wavelength light and overcoming the diffraction limit, can be used to manipulate, control and visualize optical fields on nano-meter scale [10]. Nano-antennas resonance length is considerably shorter than $\frac{\lambda}{2}$ [11, 12], where λ is the free-space incident wavelength. The optical antenna defines as a device to efficiently convert free-propagating optical radiation to localized energy, and vice versa [3]. Instead of galvanic (electric) transmission lines, localized oscillators or incident beams are often used for driving and illuminating of optical antennas [13].

By increasing applications of nano-antennas [14], efficiently harvesting of pure energy have been of particular interest [15]. Both types of surface plasmons can be used to increase absorption in solar cells. The resonance

of noble metals is often in the visible spectrum or in the area of interest for photovoltaic applications. In photovoltaic, antenna coupled diode rectifiers convert the incident electromagnetic wave to electrical signal. lumped-element and traveling wave detectors based on MIM (metal-insulated-metal) diode have studied in [16]. MIM diode in traveling wave detector is used as plasmonic waveguide.

Recently, theoretical studies focused on bowtie antennas [17] and gap antennas, due to their considerable ability of strongly enhancing and confining optical fields to sub-wavelength dimensions, surpassing the diffraction limit, and efficiently emitting the near field energy to the far field [18]. One way to achieve a broadband behavior and achieve the benefits of localized near fields [19, 20] is to develop an antenna with its symmetric structure (similar to its own). A prominent feature of the bowtie geometry is supporting multiple surface plasmon modes, facilitating field enhancement across a large bandwidth [21]. Through the field patterns in the visible light frequency spectrum, it is observed that plasmon and Fabry–Perot resonances in a bowtie antenna, depend linearly on aperture perimeter and film thickness, respectively [10].

Optical nano-antennas have great potential for numerous applications in many fields, such as nano-imaging, spectroscopy, photovoltaics [11], near field applications in biosensing [22], nanolithography [23], photo detection [24], trapping [25], heat generation [26], high-resolution microscopy and light emission tailoring [11], optoelectronic nano-device and surface enhanced Raman scattering (SERS) [27] and white light generation [19]. The most widely used methods for optical nano-antennas simulation are the finite integration technique (FIT), the finite element method (FEM) [28] and the finite difference time domain (FDTD) method [29]. In this paper we have used ACS and electric field enhancement for comparison nano-structures composed of TNP that can be useful as design and simulation guidelines for optical nano-antennas and absorbers of electromagnetic energy.

2 Simulation results and discussion

The finite integration technique (FIT), using CST microwave studio is utilized for simulations in the wavelength range of 200–1500 nm. In this article, we consider the structures consist of two, three, and four coplanar gold triangular wings that the angle between adjacent arms is 180, 120, and 90 degrees, respectively, as shown in Fig. 1a. Then, we investigate and compare the absorption cross section, absorption coefficient and the electric field enhancement of them. Figure 1b shows the prototype proposed CBNA and its geometry parameters. The structure consists of four gold triangular nano-particle placed in

Fig. 1 **a** Three investigated structures of triangular nano-particle, **b** Left panel, a three-dimensional schematic of cross bow-tie nano-antenna. Right panel, a side view and top view of the nano-antenna

close vicinity to each other in the form of cross structure. Here, we carried out a rigorous analysis and simulation of the design parameters by varying one parameter at a time (while other parameters are kept fix) and monitoring the variation of absorption cross section (ACS), absorption coefficient and electric field magnitude of the structure. The base gold triangular nano-particle (TNP) can be characterized by four structure parameters: the triangle length $a = 260$ nm, width $b = 140$ nm, thickness $t = 60$ nm and bend radius $r = 2$ nm. Johnson and Christy's material data is used for gold. The TNPs is placed on the SiO₂ layer with $\epsilon_{sub} = 2.4$ and thickness of $h = 40$ nm as a substrate and surrounding medium is vacuum with $\epsilon_{background} = 1$.

2.1 Investigation of the absorption cross section and the reflection cross section of the nano-antenna samples

When the electromagnetic waves hit the nano-structure, some of them are scattered and the rest are absorbed.

The ratio of the radiation energy absorbed by a nano-structure to the total energy radiated to it is called the absorption coefficient. Absorption cross section is a measure of the probability of an absorption process on the surface of the nano-structure. The absorption cross section, absorption coefficient and absorption spectrum of a nano-antenna depend on the incident light (wavelength, polarization and the angle of collision to nano-structure), the structure of nanoantenna (the intrinsic qualities of the material, shape, dimensions and the arrangement of the nano-particles on the nano-structure surface) and the medium surrounding the nano-antenna (the refractive index). The absorption cross section is a factor in determining the quality of nano-antenna in the absorption of incident radiation wave [30].

The nano-antenna samples are illuminated by x-polarized incident plane wave in $+z$ direction. The amplitude of the incident light is set to be 1 V/m throughout this paper. As shown in Fig. 2a, b, in the cases with 4, 6 and 8-TNP, the ACS peaks by increasing the arm number:

Fig. 2 The ACS of nano-antenna samples **a** with 2, 3 and 4-TNP arms. **b** With 4, 6 and 8-TNP arms. (for the normal incident plane wave with linear polarization in x—direction)

1. In the low wavelengths, show the same trend and have a blue shift.
2. In the high wavelengths, the peaks amplitude decrease and find the red shift.
3. The 4-TNP case also has a peak at 1200 nm in addition to the aforementioned two peaks due to vertical plasmonic resonance.

Fig. 3 The ACS and RCS of CBNA for the incident plane wave with both x-polarized and circular polarization

The electrons in the nanoparticles fluctuate with each other in response to the electric field of the incident light. The separation of charges is in the direction of the polarization of the incident electric field. Increasing the number of arm, the phase difference and scattering are more frequent and the overall absorption and peak amplitude of the absorption cross section decrease.

Gold as a noble metal has high absorption rate due to inter-band transitions in the visible and near infrared spectrum. By choosing suitable material (gold), designing and dimensions of the nano-antenna, and composition of the nano-particles on the substrate, the ACS will be greater than the reflection cross section (RCS) in entire the band (see Fig. 3). High ACS is the same what we are looking for in solar cells based on plasmonic nano-antenna.

2.2 Investigation of the absorption coefficient of the nano-antenna samples

The type of feed used in this section is the external light source through the waveguide port, as shown in Fig. 4. When the signal is coupled to the structure via port 1, some frequencies pass through the structure and collide to port 2 ($S_{2,1}$), and some frequencies do not pass through the structure and return to port 1 ($S_{1,1}$). The absorption coefficient, using scattering parameters in CST solver can be calculated as Eq. (1):

$$R = |S_{1,1}|^2, T = |S_{2,1}|^2, A = 1 - R - T \quad (1)$$

In Fig. 5, the result simulations show that the normalized absorption coefficient of CBNA, especially at visible wavelengths, is more than the other two cases. The main differences between them are the structural symmetry in the horizontal and vertical directions as well as the

Fig. 4 Feeding the structure by two waveguide ports in + z and – z direction

constructive phase difference between the resonance modes. The results confirm that the depth of penetration and thus the amount of absorption of gold in optical wavelengths are significant. Therefore, the design and material of the nano-antenna play the important role in determining the resonance points of the absorption spectra and also amount of absorption. In Fig. 6, we observe that the CBNA absorption coefficient has an acceptable distance from the reflection and transmission coefficients.

Now, we simulate the absorption, reflection and transmission coefficients of the CBNA with the Lumerical FDTD Solutions software. To do this, we illuminate the structure from the bottom of the substrate by a plane wave source. As shown in Fig. 7a, the reference planes R and T are placed at 5 nm above the structure and the bottom of the light source, respectively, to calculate

Fig. 5 The normalized absorption coefficient of three nano-antenna samples for incident waveguide port

Fig. 6 The normalized absorbance, reflectance and transmittance coefficients of CBNA for incident waveguide port

Fig. 7 **a** Top and side view of CBNA in FDTD solution environment. **b** The normalized absorbance, reflectance and transmittance coefficients of CBNA for the incident plane wave in + z direction. **c** The electric field intensity ($|E|^2$) on the x-y plane, 5 nm above the structure

reflection and transmission coefficients. Then we plot the absorption coefficient graph through the reflection and transmission data using EXCEL and MATLAB software's and apply Eq. (1), as seen in Fig. 7b. The tip of the triangular nano-particle has not bend in the FDTD Solutions environment, which makes a slight difference between the CST and FDTD Solutions results. As we expect, the intensity of the electric field in the sharp edges and corners, and especially in the center of the gap, is significantly stronger, as shown in Fig. 7c.

2.3 Investigation of the electric field enhancement of the nano-antenna samples

The normalized electric field in any point is defined in Eq. (2) as follows:

$$|E| = \frac{\sqrt{(|E_x|^2) + (|E_y|^2) + (|E_z|^2)}}{E_i} \quad (2)$$

where E_x , E_y and E_z are the x, y and z components of the electric field, E_i is the amplitude of the electric field of the incident light source. According to the definition, $|E|$ is dimensionless quantity represents the magnitude of the enhancement of the electric field at any point [31]. It can be seen from Figs. 8 and 9 that the increasing of the CBNA electric field for both linear x-polarized and circular polarization of incident plane wave has two constant resonances, with the difference that the amplitude of $|E|$ in the circular polarization has doubled from the structural symmetry in the direction x and y are obtained. The nano-antenna sample with two TNP arms has the strongest and lowest electric field enhancement with x-polarized and circular polarization of incident light, respectively, because it is not possible to create a near field with circular polarization using a two-arm nano-antenna. These types of nano-antennas are coupled by a component of the light coming down along the nano-antenna axis and produce linear polarization. The other vertical component that needed to form a circular polarization is not produced in this process.

The results of the illumination of the CBNA are identical with the incident plane wave with different linear polarization angles (ϕ), as shown in Fig. 10. From the results in Figs. 8, 9 and 10, it is found that the CBNA is suitable for linear and circular polarization.

2.3.1 Effect of the material properties of the TNP

Metals exhibit very different electromagnetic properties at optical frequencies. According to information [10], the

skin depths of aluminum, gold, silver and copper in the visible and near-infrared frequencies are as follows:

$$(\text{skin depth})_{Cu} > (\text{skin depth})_{Au}, (\text{skin depth})_{Ag} > (\text{skin depth})_{Al}$$

Noble metals such as gold, silver, and copper have good absorption rates in the visible frequencies. Electrons are excited by energy absorption from the high bands below the Fermi surface and this increases the imaginary part of ϵ . Therefore, the coupling between photons and electrons that result in plasmonic waves is significant in these metals. However, in metal nano-structures made of aluminum, platinum and beryllium, surface plasmon excitation is not observed. The skin depth of the metal is defined as Eq. (3):

$$\delta = \frac{\lambda}{2\pi k} \quad (3)$$

where k is absorption coefficient of the metal and λ is the wavelength. In visible and near-infrared regime, the Eq. (3) approximate to:

$$\delta = \frac{c}{\omega_p} \quad (4)$$

where ω_p is the plasma frequency and c is the velocity of light. Therefore, the resonance wavelength decreases inversely with the increasing plasma frequency of the metal and so increases nearly linearly with increasing skin depth of the metal of nano-antenna [10], as shown in Fig. 11.

Fig. 8 The electric field enhancement of three nano-antenna samples illuminated by incident plane wave **a** with x-polarized, **b** with circular polarization

Fig. 9 The electric field enhancement of three nano-antenna samples illuminated by x-polarized and circular incident plane wave

2.4 Effect of the embedding depth of the TNP in the substrate

As depicted in Fig. 12b, the increasing of embedding depth (but until the especial depth) of CBNA in a silica substrate, causes a red-shift toward longer wavelengths. The effects of substrate polarization, as well as the interaction between the TNPs and the applied incident field, make these changes [32].

2.5 Effect of the material properties of the substrate

The electric dispersion of gold is illustrated by the Johnson and Christy's material data in Fig. 13a. The real part changes of the dielectric function of the gold are nonlinear for values smaller than -5.3 . For $\mu = 1$, By increasing the refractive index of the substrate material (ϵ_{sub}) from 1

to 2.65, the resonance peaks shift to longer wavelengths but for $\epsilon_{sub} > 2.65$ where, ($\epsilon_{gold} = -5.3 = -2\epsilon_{sub}$) result in nonlinear variation, as shown in Fig. 13b.

2.6 Effect of the background of the antenna

For $\mu = 1$, By increasing the refractive index of the medium surrounding the antenna ($\epsilon_{background}$), the resonance peak shifts slightly to longer wavelengths but while $\epsilon_{background} > 2.65$ where, ($\epsilon_{gold} = -5.3 = -2\epsilon_{background}$) this order is absent, as shown in Fig. 14.

2.7 Two-dimensional array of the proposed CBNA

As we see in Fig. 15, for the 3×3 array of CBNA, with increasing center-to-center spacing of adjacent cells, from 560 to 700 nm, the amplitudes of both resonance peaks increase simultaneously, but when this distance is greater

Fig. 10 **a** The incident plane wave with different linear polarization angle(ϕ). **b** The electric field enhancement of CBNA for different ϕ

Fig. 11 The electric field enhancement for different metals used in CBNA structure for the incident plane wave with circular polarization

Fig. 12 **a** Side view of the CBNA with different embedding depths in a silica substrate. **b** The electric field enhancement for different embedding depths of the CBNA structure in the substrate for the incident plane wave with circular polarization

than 700 nm, the resonance peak amplitude with shorter wavelength decreases, but the resonance peak amplitude with longer wavelength increases.

3 Conclusions

The nano-antennas that used in solar cells, should capable to absorbing energy in the visible and infrared wavelengths and have a slight sensitivity to polarization, because the input electromagnetic signals have not selective polarization. In this study, we have designed the nano-antenna structure with suitable absorption cross section, absorption coefficient and electric field enhancement in the visible and near-infrared spectrum. The proposed nano-antenna can perform the same function when the incident light polarization is along the horizontal or vertical arm, due to its structure symmetry. Cross structure is chosen for the nano-antenna that its symmetrical shape is an important parameter for some applications, such as solar cells and optical devices.

Fig. 13 **a** The electric dispersion of gold based on Johnson and Christy's material data. **b** Influence of the material properties is used as substrate (for circular polarization)

Fig. 14 The electric field enhancement for the different medium surrounding the CBNA (for circular polarization)

Fig. 15 The electric field enhancement of the 3×3 array of the CBNA for circular polarization incident plane wave

Compliance with ethical standards

Conflict of interest The authors declare that they have no conflict of interest.

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