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Polarizability Tensor Calculation Using Induced Charge and Current Distributions

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Abstract—We develop a semi-analytical approach to calculate the polarizability tensors of an arbitrary scatterer. The approach is based on numerical integration from induced charges and currents on the scatterer. By taking the advantages of the present approach, we calculate the polarizability tensors of any arbitrary scatterer in a homogeneous isotropic medium. This approach, in comparison to other reported approaches, is simple, easily implemented, and does not require spherical harmonic expansion or complicated far-field calculations. We examine the validity of the approach using several examples and compare the results with other approaches.

1. INTRODUCTION

The electromagnetic response of composite materials, including metamaterials, mainly depends on two important factors: 1) the properties of their "constituent elements"[†] and 2) the manner in which these elements are arranged together. The latter determines the interaction effects between the elements while the former demonstrates the general response of elements. Indeed, the electromagnetic behaviour of the constituent elements may be described by the polarizability tensors [1]. Polarizability tensors determine the relation between the induced dipole moments and the external electromagnetic field excitation for a particle with linear response to the fields [2]. We may sufficiently explain the electromagnetic behaviour of many small particles by their dipolar moments or equivalently their polarizability tensors. Therefore, various *analytical* and *numerical* approaches have been employed to calculate the polarizability tensors of different particles [3–7].

For instance, the polarizability of a dielectric sphere is analytically calculated in [8]. Moreover, analytic formulas are derived for polarizabilities of wire dipole [2], chiral [3], and Ω-shaped particles [9]. Furthermore, the polarizabilities of two nonreciprocal magnetic particles; i.e., Tellegen-omega and "moving"-chiral are formulated in [4]. These analytical approaches are not only difficult but also limited to simple structures. Moreover, small modifications to the particle structure result in a different analytical model.

Consequently, for more complicated shapes, different semi-analytical and numerical methods have been proposed [5–7, 10]. For example, Alaee et al. derived the polarizabilties of a planar omega structure using multipole moments approach [5]. Their method was based on the expansion of spherical harmonics of the Mie coefficients [11] in the Cartesian coordinate system. The main disadvantage of this method is the cumbersome calculation of the spherical harmonics.

Recently, another numerical method is developed to retrieve the polarizability tensors of general bianisotropic particles [12]. It directly calculates the induced dipole moments of an excited scatterer and does not require complicated calculations and harmonic expansions. In this method, one probes the scattered far-fields of an excited particle and relates them to the radiation effects of a pair of electric

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[†] Also, called "inclusion", "scatterer", or "particle" in the current manuscript. It is called "meta-atom" in metamaterials.

and magnetic dipole moments. This method is based on the assumption of predominantly dipolar resonances and neglecting higher order multipoles. Therefore, if higher order multipoles of the scatterer are comparable to its dipolar terms, this method gives wrong results.

To overcome all the above deficiencies, we develop a method to calculate the polarizability tensors of a general bianisotropic particle. This method is based on the calculation of the near field response of a particle to the plane wave illumination. We numerically integrate from induced charges/currents on the particle to determine multipole moments and consequently the polarizability tensors. This way we provide an approach in which it adds the strength of different reported semi-analytical approaches in [5, 12][‡].

Hence, the paper is organized as following. The second section introduces our approach: the general ideas, formulation and numerical test set-up. It provides the procedure of evaluating polarizability tensors for an arbitrary isolated particle in a homogenous host medium such as free space. After presenting the analytical framework, in the third section, the proposed method is verified using various examples.

In the third section, we start with the calculation of polarizability tensors of a chiral particle in free space and then compare the results with the analytical method presented in [3] as well as the scattered far-field method presented in [12]. Next, we examine a non-reciprocal Tellegen-omega particle and compare its polarizabilities with those presented in [4]. Thereafter, we calculate the polarizability tensors of a nano-gold split ring resonator to demonstrate the capability of our proposed method in the terahertz frequency region. We also show that the higher order multipoles of such structure are negligible compared to its dipole moments. This is impossible to demonstrate with the presented method in [12]. Finally, in the last section we conclude the study.

2. THEORY

We present a procedure for retrieval of the polarizability tensors of an arbitrary scatterer in a homogeneous host medium. The parameters which connect the induced electric and magnetic dipole moments $\mathbf{p}$ and $\mathbf{m}$ to the "local" electric and magnetic fields $\mathbf{E}^{\text{loc}}$ and $\mathbf{H}^{\text{loc}}$ are called polarizabilities. These relations may be summarized in the following compact forms [2]:

$$\begin{bmatrix}\mathbf{p}\\ \mathbf{m}\end{bmatrix} = \begin{bmatrix}\bar{\bar{\alpha}}^{\text{ee}} & \bar{\bar{\alpha}}^{\text{em}}\\ \bar{\bar{\alpha}}^{\text{me}} & \bar{\bar{\alpha}}^{\text{mm}}\end{bmatrix}\begin{bmatrix}\mathbf{E}^{\text{loc}}\\ \mathbf{H}^{\text{loc}}\end{bmatrix}. \tag{1}$$

Here $\bar{\bar{\alpha}}^{\text{ee}}$, $\bar{\bar{\alpha}}^{\text{mm}}$, $\bar{\bar{\alpha}}^{\text{em}}$, and $\bar{\bar{\alpha}}^{\text{me}}$ are the electric, magnetic, magnetoelectric, and electromagnetic polarizability tensors, respectively. In a three-dimensional coordinate system, each of these polarizability tensors has nine components. Therefore, in order to completely characterize a particle response to an electromagnetic wave, there are 36 polarizability components that should be calculated.

Let us first consider a particle in the origin of the Cartesian coordinate system in a homogeneous host medium with the intrinsic impedance η as shown in Fig. 1. Now let us start with the calculation of $\alpha^{\text{ee}}_{\text{ix}}$, and $\alpha^{\text{me}}_{\text{ix}}$ where $\text{i} = \text{x}, \text{y}, \text{z}$. According to Ref. [10] and Equation (1), we should determine the particle response ($\mathbf{p}_i$ and $\mathbf{m}_i$) to an x-directed exciting electric field. To create such an electric field, we apply two oppositely plane waves which are traveling in the z-direction with similar polarizations for their electric fields (green color vectors in Fig. 1); i.e., $E^{\pm}_x = E_0 e^{j(\omega t \mp kz)}$, where ω and k are the angular frequency and wavenumber, respectively[§]. Notice, $\pm$ sign in the superscript refers to the propagation in $\pm z$-direction. Since the two magnetic fields are out of phase, then summing these two plane waves copies a standing wave with an electric-field maximum and a magnetic-field zero at the place of the particle assuming the particle is small compared to the wavelength. As a result, the polarizabilities can be easily calculated as:

$$\alpha^{\text{ee}}_{\text{ix}} = \frac{\text{p}^{+}_{\text{i}} + \text{p}^{-}_{\text{i}}}{2E_0}, \quad \alpha^{\text{me}}_{\text{ix}} = \frac{\text{m}^{+}_{\text{i}} + \text{m}^{-}_{\text{i}}}{2E_0}. \tag{2}$$

Here, the $\pm$ sign in the superscript of the dipole moments, denotes the induced moment by the corresponding plane wave in $\pm z$-direction. In a similar way, subtracting these two plane waves creates

‡ That is, calculation of higher order multipoles as well as the polarizability retrieval of general bianisotropic particles.
§ We consider the time dependence $e^{j\omega t}$ all over the manuscript

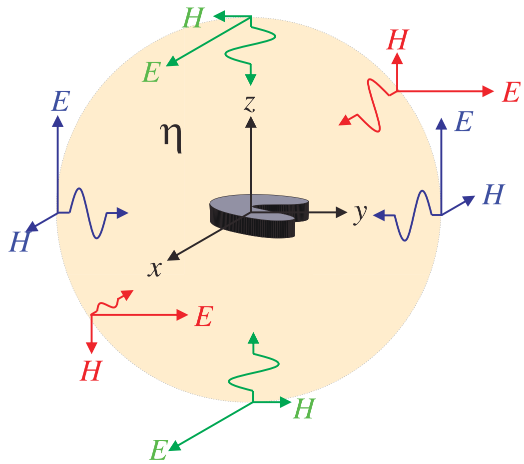


Figure 1. Polarizability tensor extraction setup: an arbitrary scatterer is located in the origin of the coordinates and is illuminated by six orthogonal plane waves.

a local maximum of the magnetic field with zero electric field. Therefore, one can write

$$\alpha_{\mathrm{iy}}^{\mathrm{em}} = \frac{\mathrm{p}_{\mathrm{i}}^{+} - \mathrm{p}_{\mathrm{i}}^{-}}{2E_0}\eta, \quad \alpha_{\mathrm{iy}}^{\mathrm{mm}} = \frac{\mathrm{m}_{\mathrm{i}}^{+} - \mathrm{m}_{\mathrm{i}}^{-}}{2E_0}\eta. \tag{3}$$

We should mention again that the exciting field is assumed to be a constant value in the place of the particle. This is true when the size of the particle is sufficiently smaller than the operating wavelength.

One may obtain 12 polarizabilty components from Equations (2) and (3). Other components may be calculated similarly with $E_y^{\pm} = E_0 e^{j(\omega t \mp kx)}$ and $E_z^{\pm} = E_0 e^{j(\omega t \mp ky)}$ as the excitation electromagnetic wave (red color and blue color vectors in Fig. 1). So far, we expressed that six orthogonal plane waves are needed to calculate all polarizability components. Moreover, we built the relations between polarizability components and the dipole moments. In the next step, we present how the required dipole moments may be calculated from the induced currents and/or charges [13].

When an electromagnetic field illuminates a particle, the equilibrium of charges (either free charges or bounded ones) in/on the particle is changed. This excited particle can be modelled as an expansion of multipole moments. The first four successive electric multipole moments in terms of the induced charge density $\rho(\mathbf{r})$ are expressed as [13]

$$\begin{aligned} \mathrm{q} &= \int_V \rho(\mathbf{r})dv, \quad \mathrm{p}_{\mathrm{i}} = \int_V r_{\mathrm{i}}\rho(\mathbf{r})dv, \\ \mathrm{q}_{\mathrm{ij}} &= \int_V r_{\mathrm{i}}r_{\mathrm{j}}\rho(\mathbf{r})dv, \end{aligned} \tag{4}$$

where V is the volume of the particle and r the position vector in the Cartesian coordinate system. Subscripts $\mathrm{i, j, k}$ denote components of a Cartesian tensor, and q, p_{i}, and q_{ij} are the electric monopole, dipole, and quadrupole moments, and so forth, respectively. Since the total electric charge of the particle after the illumination remains zero, we have: $q = 0$.

Similarly, the first two magnetic multipole moments are expressed in terms of the induced current density $\mathbf{J}(\mathbf{r})$ as:

$$\begin{aligned} \mathrm{m}_{\mathrm{i}} &= \tfrac{1}{2}\textstyle\int_V (\mathbf{r} \times \mathbf{J}(\mathbf{r}))_{\mathrm{i}}dv, \\ \mathrm{m}_{\mathrm{ij}} &= \tfrac{2}{3}\textstyle\int_V (\mathbf{r} \times \mathbf{J}(\mathbf{r}))_{\mathrm{i}}r_{\mathrm{j}}dv, \end{aligned} \tag{5}$$

where m_{i} and m_{ij} are the magnetic dipole and quarupole moments, respectively. Finally, we may summarize our procedure for calculating polarizability tensors as following. First, we simulate the scatterer which is illuminated by three couples of plane waves in three orthogonal directions. Then, using numerically calculated dipole moments (Equations (4), (5)), we easily find the polarizability tensors components from Equations (2) and (3).

In the next section, we focus on different examples to validate our semi-analytical approach in calculation of the polarizability tensors. In the beginning, we calculate the polarizability tensors of a chiral particle at microwave frequencies.

3. RESULTS AND DISCUSSION

3.1. Wire Chiral Particle

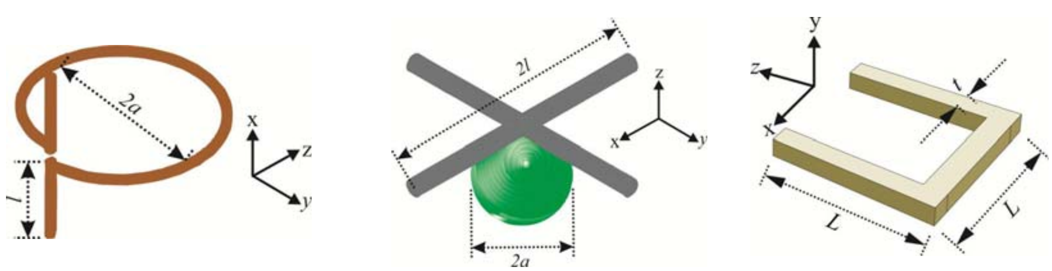
One of the interesting bianisotropic particles with a variety of applications in the field of electromagnetics is "chiral" particle [14–16]. A chiral is an object which can be distinguished from its mirror image and cannot be superposed onto it [17]. A typical wire chiral particle is shown in Fig. 2(a). It is composed of a planar loop connected to two straight wires orthogonal to the loop plane. According to the coordinates of Fig. 2(a), this chiral particle provides the following ten major polarizability components

$$\begin{aligned}
&\bar{\bar{\alpha}}^{\mathrm{ee}} \cong \alpha_{xx}^{\mathrm{ee}}\hat{\mathbf{x}}\hat{\mathbf{x}} + \alpha_{xy}^{\mathrm{ee}}\hat{\mathbf{x}}\hat{\mathbf{y}} + \alpha_{yx}^{\mathrm{ee}}\hat{\mathbf{y}}\hat{\mathbf{x}} + \alpha_{yy}^{\mathrm{ee}}\hat{\mathbf{y}}\hat{\mathbf{y}} + \alpha_{zz}^{\mathrm{ee}}\hat{\mathbf{z}}\hat{\mathbf{z}},\\
&\bar{\bar{\alpha}}^{\mathrm{mm}} \cong \alpha_{xx}^{\mathrm{mm}}\hat{\mathbf{x}}\hat{\mathbf{x}},\\
&\bar{\bar{\alpha}}^{\mathrm{em}} \cong \alpha_{xx}^{\mathrm{em}}\hat{\mathbf{x}}\hat{\mathbf{x}} + \alpha_{yx}^{\mathrm{em}}\hat{\mathbf{y}}\hat{\mathbf{x}},\\
&\bar{\bar{\alpha}}^{\mathrm{me}} \cong \alpha_{xx}^{\mathrm{me}}\hat{\mathbf{x}}\hat{\mathbf{x}} + \alpha_{xy}^{\mathrm{me}}\hat{\mathbf{x}}\hat{\mathbf{y}}.
\end{aligned} \tag{6}$$

Other polarizability components are negligible or zero compared to these components. Moreover, from the reciprocity we have

$$\bar{\bar{\alpha}}^{\mathrm{ee}} = (\bar{\bar{\alpha}}^{\mathrm{ee}})^{\mathrm{T}}, \quad \bar{\bar{\alpha}}^{\mathrm{mm}} = (\bar{\bar{\alpha}}^{\mathrm{mm}})^{\mathrm{T}}, \quad \bar{\bar{\alpha}}^{\mathrm{em}} = -(\bar{\bar{\alpha}}^{\mathrm{me}})^{\mathrm{T}}. \tag{7}$$

In [3], a wire and loop model is used to analytically calculate the chiral polarizabilities in terms of the model parameters. We choose a wire chiral example with the radius $a = 1.7$ mm and an arm length of $l = 1.1$ mm which provides a resonant response around 10 GHz. The polarizabilities of this particle are calculated using three methods: induced currents (our proposed method), the wire and loop model presented in [3], and the scattered far-field method proposed in [12]. The results are depicted in Fig. 3. As can be seen from Fig. 3, the results of our method coincide with those of scattered far-field method [12]. Moreover, the wire and loop model results in an accurate prediction of the resonance frequency while it does not precisely foretell about the strength of the polarizabilities at resonance. The difference is due to the fact that a chiral particle is not exactly a combination of a wire and a loop as considered in [3]. Indeed, they interact together which is neglected in that model. Notice, all results respect the reciprocity theorem through Equation (7). Note also the different resonant frequencies of $\alpha_{zz}^{\mathrm{ee}}$ with other polarizability components. This is due to the smaller resonant length of the particle in the z direction.



(a) (b) (c)

Figure 2. The scatterers under study: (a) A wire chiral with radius of a and arm length of l, the radius of wire is r_0, (b) a Tellegen-Omega particle composed of two crossed PEC wires with total length of $2l$ on top of a ferrite sphere with radius of a, the ferrite sphere is biased along z-axis, (c) a split ring resonator with an arm length of L and the thickness of t.

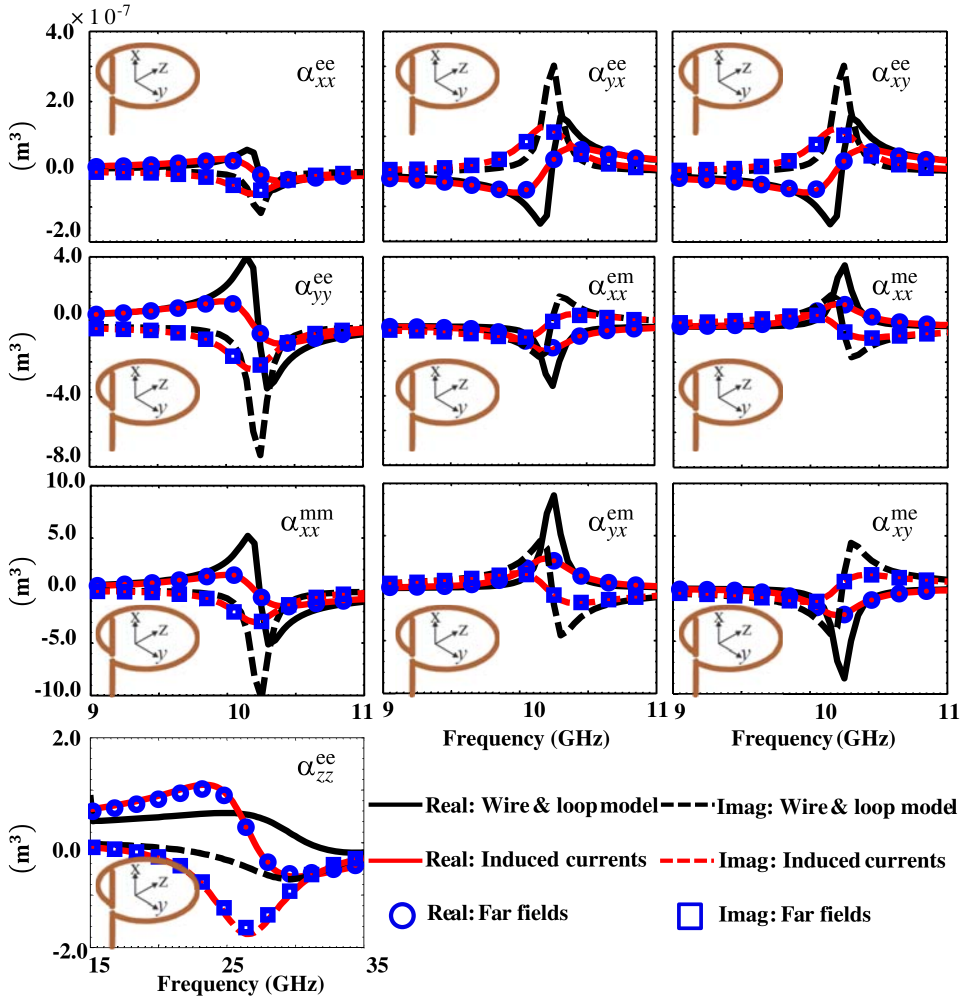


Figure 3. The major polarizability components of the chiral element shown in Fig. 2 which are calculated by the proposed method and compared to the wire and loop model as well as the far-field method.

3.2. Non-Reciprocal Tellegen-Omega Particle

Nonreciprocal particles and their applications are comprehensively discussed in [1]. These particles may be realized using a biased magnetic element (e.g., ferrites) and some conducting wires. Two famous examples are Tellegen-omega/"moving"-chiral particles which simultaneously presents the properties of Tellegen and omega/"moving" and chiral bianisotropies, respectively. A Tellegen-omega particle as shown in Fig. 2(b) may be composed of a ferrite sphere and two orthogonal wires. When an incident electric field excites one of the wire arms, the induced electric current will produce two crossed magnetic moments in the ferrite sphere which in turn they induce currents on the wires. From the symmetry of the structure with respect to the x and y axes, one can deduce that

$$\begin{aligned} \alpha_{xx}^{\mathrm{ee/mm/me/em}} &= \alpha_{yy}^{\mathrm{ee/mm/me/em}}, \\ \alpha_{xy}^{\mathrm{ee/mm/me/em}} &= \alpha_{yx}^{\mathrm{ee/mm/me/em}}. \end{aligned} \tag{8}$$

We calculated the major polarizability components of the structure using the presented method of *induced currents* and compared them with the method of scattered far-field presented in [12]. The results are shown in Fig. 4. Again, for this non-reciprocal element, the results of our proposed method coincide with the scattered far-field results. This proves the power of our method in calculation of the polarizabilities of non-reciprocal particles.

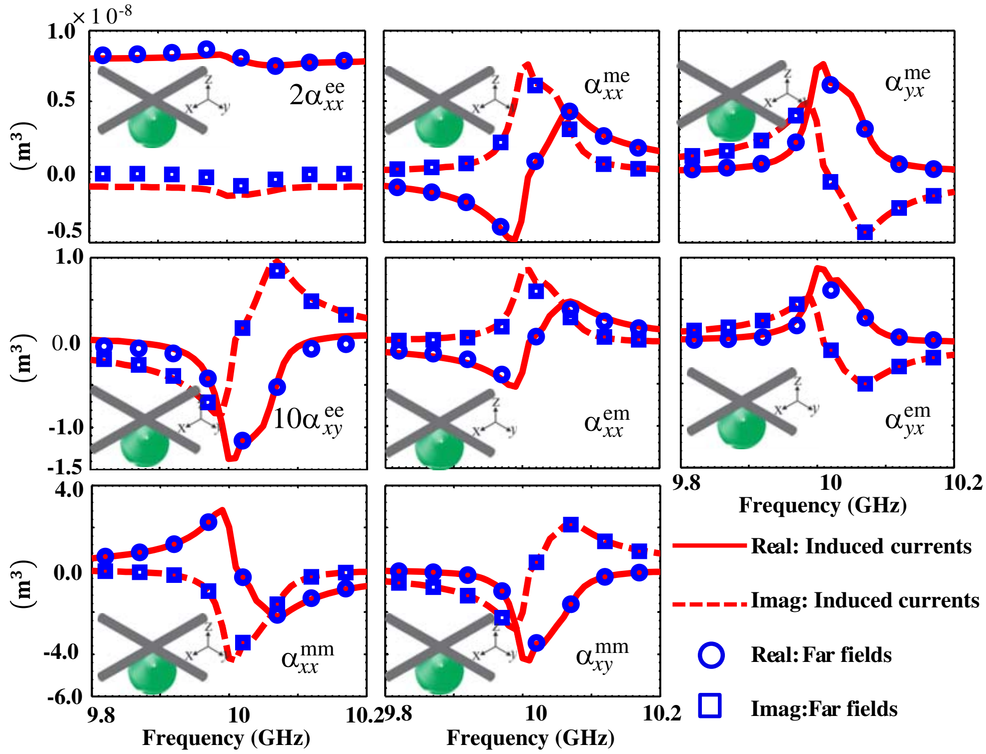


Figure 4. Major polarizabilities of the Tellegen-Omega particle of Fig. 2(b) calculated through proposed method and compared to far-field approach. The properties and dimensions of the particle are: $l = 1\,\text{mm}$, $a = 0.5\,\text{mm}$, Ferrite material: YIG with relative permittivity $\epsilon_r = 15$ and magnetic saturation $M_s = 1780\,\text{G}$. The applied bias field is 3000 Oe.

The next example is associated with the calculation of the polarizabilities of an artificial optical magnetic dipole; that is, a nano-gold split-ring resonator (SRR).

3.3. Split Ring Resonator

Split ring resonators (SRRs) are widely used in terahertz frequencies since they provide artificial magnetism which is naturally prohibited at these high frequencies [18]. A typical SRR is depicted in Fig. 2(c). Its magnetic moment is created in y direction due to a circulating current in the SRR arms. This current may be induced by an electromagnetic plane wave illumination.

The main polarizability components of the proposed SRR are calculated using our method of *induced currents* and are compared with the method of scattered far-field presented in [12]. The results are shown in Fig. 5. As can be seen from the figure, the results of the proposed method coincides with the results extracted from the approach of the scattered far-field. Therefore, one may deduce that the SRR can be replaced with an electric and a magnetic dipole.

At this step, we clarify an important issue concerning the calculations of higher order multipoles. It is impossible to investigate the effect of higher order multipoles using the method proposed in Ref. [12] from the scattered far fields. Moreover, to calculate higher order multipoles by the expansion of spherical harmonics using the scattered fields one requires to solve a complicated problem as the order increases (e.g., see in Ref. [19]). However, since in our proposed method we are numerically integrating from the induced charges/currents over the particle, then we may directly calculate higher order multipoles up to any desired order without increasing the problem complexities. A common way to investigate the effect of higher order multipoles is to compare the effect of different multipole moments in the scattering cross section of the particle [19]. As the orders of multipoles increase their contributions in the scattering cross section decrease. Here, we compare the effect of strongest electric (p_x) and magnetic dipole moments (m_y) with the strongest electric quadropole moment (Q_{xz}) in Fig. 6(a).

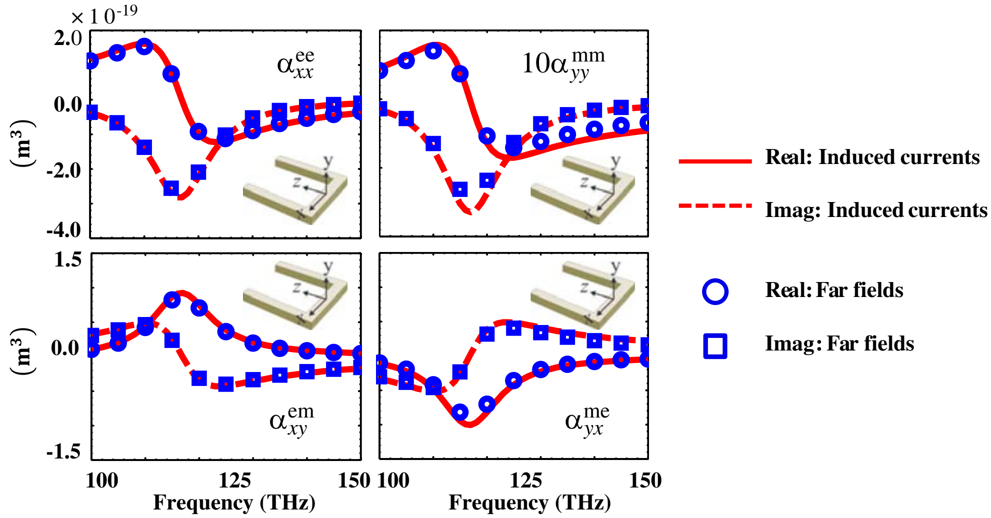


Figure 5. The major polarizabilities of the proposed split ring resonator. Comparison of our method with the far-field method. The length and the thickness of the SRR are $L = 300$ nm and $t = 40$ nm while it is made of gold in which its dispersive material parameters are taken from [20].

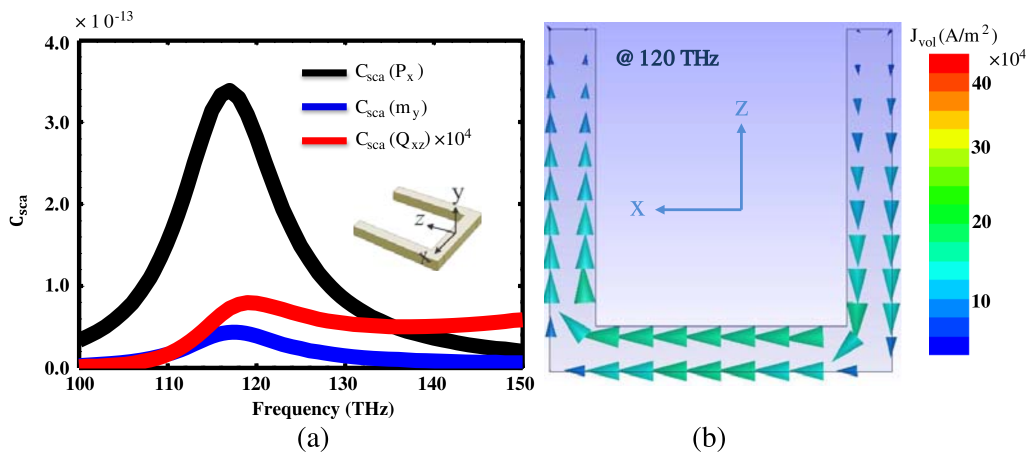


Figure 6. (a) Scattering cross sections due to the different multipole moments of the SRR, (b) induced current distribution on the SRR at resonance frequency 120 THz.

As can be seen from this figure, the effect of quaropole moments are negligible. It is an important fact that we may investigate directly using our proposed method of induced currents. Moreover, from the induced current distribution on the SRR in Fig. 6(b), it can be easily seen that the SRR provides a strong electric dipole in x direction (p_x). Furthermore, a circulating current in the SRR arms results in a magnetic dipole in y direction (m_y). So, the SRR can be effectively modelled as a pair of electric and magnetic dipole (p_x/m_y). This way we may have a fast physical insight of the complexity of a desired particle. Indeed, without this analysis, it is impossible to consider a particle as dipoles only. As a result, our proposed method not only provides the polarizabilities of any kind of dipole particles but also presents a very useful and powerful physical insight of any general particle. More importantly, we do not need extra calculations to grasp such physical insight. Therefore, we gain too many information with a simple method.

4. CONCLUSION

We developed a method for the calculation of polarizability tensors of any arbitrary isolated scatterer. In this method, we used induced charges/currents of the particle excited by plane waves. The method does not require complicated calculations and harmonic expansions. We expressed different examples (wire chiral, Tellegen-omega, and SRR) and calculated their polarizability tensors. The results were in quite good agreement with other available methods. We showed how this method present a physical insight of each design and to what extend one may use the concept of dipole model. By presenting different examples, we have shown that this method can be applied to arbitrary scatterers with arbitrary shapes and materials (dispersive, non-reciprocal, etc.), and also for one part as well as multi parts scatterers.

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