 

***METAMATERIALS***

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# Analysis of optical properties of planar metamaterials by calculating multipole moments of their constituent meta-atoms

A.A. Pavlov, V.V. Klimov, Yu.V. Vladimirova, V.N. Zadkov

***Abstract.*** **On the basis of calculations of multipole moments of meta-atoms forming a planar metamaterial, a new method is proposed for the quantitative determination of its optical and polarisation properties. The efficiency of the method is demonstrated by the example of a planar metamaterial consisting of H-shaped nanoparticles.**

***Keywords:*** *metamaterials, planar metamaterials, nanoparticles, far fields.*

## 1. Introduction

The optical properties of 'unique' materials – metamaterials – have been the subject of active research in recent years [1]. Metamaterials are artificially engineered materials composed of nanoparticles (meta-atoms) which are arranged at nanometre distances from each other and play the role of ordinary atoms. Such materials can have a number of properties not inherent in conventional materials, and therefore, arouse great interest. The main feature of metamaterials is the 'decoupling' of electric and magnetic properties of nanoparticles, because at the nanoscale Maxwell's equations for the electric and magnetic fields become independent due to the absence of delay. It is this fact that makes it possible to produce metamaterials with virtually arbitrary optical properties and to make use of them to control light at the nanoscale. Based on metamaterials there have already been designed or are being developed super- and hyperlenses, near-field sensors, ideal photon detectors and a variety of other devices [1–6].

Among the variety of metamaterials we should single out planar metamaterials that consist of one or more flat layers of nanoparticles. The importance of such materials is caused by both the relative simplicity of manufacture and the ability to integrate with modern silicon electronics. These features of planar metamaterials have even led to the birth of a new term, i.e., 'flat nanophotonics'.

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In attempting a theoretical description of the optical properties of metamaterials, there arise considerable difficulties due to the complex shape of the constituent meta-atoms, as well as due to the fact that a significant role at the nanoscale is played by longitudinal near fields, which are impossible to describe analytically in most cases. Analytical expressions for the scattered field in the general form can be derived only for the wave scattered on single spherical, spheroidal and ellipsoidal nanoparticles [2]. In all other cases, the problem must be solved numerically; however, because the modelling domain is always limited in space, one can only realistically calculate the near fields, and far fields, which are important for practical applications, are left out of consideration.

There are various numerical methods which allow one to calculate electric and magnetic fields of metamaterials. The widely used methods are the finite difference time domain (FDTD) method and discrete dipole approximation (DDA) (a detailed description of these and other numerical methods is given in [2]). However, these methods have some drawbacks. Thus, the efficiency of the FDTD method is hampered by the need for a large amount of rapid access memory, as well as the complexity of the description of materials with dispersion (metals) at oblique incidence of light on the plane of the metamaterial. When using the DDA, more problems arise. First, its convergence has not been proved, and the accuracy of better than a few percent is rarely attainable. Second, near fields in this method are not evaluated and, apparently, cannot be calculated correctly. Far fields are also not fully evaluated, as their section only can be determined. For these reasons, to model the interaction of an electromagnetic wave with a metamaterial, we used the COMSOL Multiphysics package to calculate the fields in the near zone by the finite element method (FEM).

In this paper, we demonstrate the possibility of a quantitative description of the optical properties of a planar metamaterial, consisting of nanoparticles of arbitrary shape, by calculating numerically the multipole moments of the particles and determining analytically the far fields. The geometry of the problem is shown in Fig. 1.

In Section 2 we set forth the essence of our method. The main idea is to represent the currents induced by the incident electromagnetic wave inside the nanoparticles in the form of oscillating multipoles generating a scattered field. Using these multipole moments we can derive analytical expressions for the scattered field, thereby making it possible to determine the properties of the transmitted and reflected waves in the far field, as well as to compute the Stokes parameters, which is of interest for the study of metamaterials consisting of chiral nanoparticles. In Section 3 we demonstrate the effectiveness of our method for studying the optical and polarisation prop-

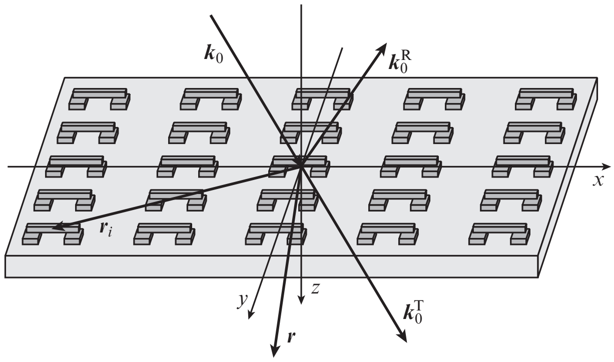


**Figure 1.** Schematic view of the planar metamaterial under study.

erties of a planar metamaterial composed of H-shaped nanoparticles (an experimental study of the metamaterial is given in [7]). In particular, we calculate the Stokes parameters and draw a conclusion about the conversion efficiency of the incident wave polarisation by this metamaterial.

## 2. Calculation of far fields by multipole moments of meta-atoms

To describe the optical properties of metamaterials by using multipole moments of meta-atoms, we will use the integral expression for the scattered field [8]:

$$\boldsymbol{E}_{\mathrm{sc}} = \mathrm{rot\,rot}\int \frac{\varepsilon(\boldsymbol{r}') - 1}{4\pi} \frac{\boldsymbol{E}(\boldsymbol{r}')\exp(\mathrm{i}k_0 R)}{R}\mathrm{d}V', \quad (1)$$

where $\boldsymbol{E}$ is the electric field vector within the particle; $k_0$ is the modulus of the wave vector of the incident wave; $R = |\boldsymbol{r} - \boldsymbol{r}'|$; $\boldsymbol{r}$ is the radius vector of the observation point; $\boldsymbol{r}'$ is the radius vector of the element with the volume $\mathrm{d}V'$; $\varepsilon$ is the relative permittivity of the particle; and the integration is performed over the volume of the metamaterial. Using the value of the field inside the particles found by the numerical simulation methods, this expression allows one to find the scattered (i.e., far) fields, and thus describe the 'external' properties of the metamaterial.

We now use (1) to describe the scattering by a plane monochromatic wave $\boldsymbol{E}_0(\boldsymbol{r}, t) = \boldsymbol{E}_0\exp(\mathrm{i}\boldsymbol{k}_0\boldsymbol{r})\exp(-\mathrm{i}\omega t)$ on a planar metamaterial consisting of periodically arranged meta-atoms of arbitrary shape. Below, the time-dependence factor will be omitted. Let $\boldsymbol{r}_i$ be the radius vector of the $i$th particle with respect to the zero particle located at the origin of the coordinates. Then, using only the smallness of the nanoparticle size as compared with the wavelength, we obtain from expression (1) the expressions for the scattered field generated by an infinite plane of particles as the sum of the individual particles:

$$\boldsymbol{E}_{\mathrm{sc}}(\boldsymbol{r}) = \frac{1}{4\pi\varepsilon_0}\mathrm{rot\,rot}\sum_i \exp[\mathrm{i}(\boldsymbol{k}_0\boldsymbol{r}_i)] \times \frac{\exp[\mathrm{i}k_0|\boldsymbol{r} - \boldsymbol{r}_i|]}{|\boldsymbol{r} - \boldsymbol{r}_i|}(\boldsymbol{d} - \mathrm{i}k_0\hat{\boldsymbol{M}}\boldsymbol{n}_i), \quad (2)$$

where

$$\boldsymbol{d} = \varepsilon_0\int(\varepsilon(\boldsymbol{r}') - 1)\boldsymbol{E}(\boldsymbol{r}')\mathrm{d}V' \quad (3)$$

is the vector of the electric dipole moment of the particle located at the origin of the coordinates;

$$\hat{\boldsymbol{M}}\boldsymbol{n} = \varepsilon_0\int(\varepsilon(\boldsymbol{r}') - 1)\boldsymbol{E}(\boldsymbol{r}')(\boldsymbol{n}\boldsymbol{r}')\mathrm{d}V' \quad (4)$$

is the projection vector of the tensor $\hat{\boldsymbol{M}}$ of the combined magnetic dipole and electric quadrupole moments of the zero particle in the direction $\boldsymbol{n}$; $\boldsymbol{n}_i = (\boldsymbol{r} - \boldsymbol{r}_i)/|\boldsymbol{r} - \boldsymbol{r}_i|$ is the unit vector of the observation point from the $i$th particle. In (3) and (4) integration is performed over the volume of the nanoparticles positioned at the origin of the coordinates.

Consider now the terms that contain the electric dipole moment $\boldsymbol{d}$. Assuming the distance between the nanoparticles to be much smaller than the wavelength (which by definition is valid for metamaterials), the summation over the particles can be replaced by integration over an infinite plane. As a result, the expression for the far field of an infinite plane grating of nanoparticles taking into account only the electric dipole moment will have the form:

$$\boldsymbol{E}_{\mathrm{sc}}^{\mathrm{d}} = -\frac{\mathrm{i}}{2\varepsilon_0 k_{0z}\Delta S}\exp[\mathrm{i}(\boldsymbol{k}_0'\boldsymbol{r})][\boldsymbol{k}_0'[\boldsymbol{k}_0'\boldsymbol{d}]],$$

$$\boldsymbol{H}_{\mathrm{sc}}^{\mathrm{d}} = \frac{\mathrm{i}}{2\varepsilon_0 Z_0 k_0 k_{0z}\Delta S}\exp[\mathrm{i}(\boldsymbol{k}_0'\boldsymbol{r})][\boldsymbol{k}_0'[\boldsymbol{k}_0'[\boldsymbol{k}_0'\boldsymbol{d}]]], \quad (5)$$

where $\boldsymbol{k}_0' = \boldsymbol{k}_0^{\mathrm{T}} = \boldsymbol{k}_0 = (k_{0x}, k_{0y}, k_{0z})$ for the transmitted wave and $\boldsymbol{k}_0' = \boldsymbol{k}_0^{\mathrm{R}} = (k_{0x}, k_{0y}, -k_{0z})$ for the reflected wave; $Z_0 = \sqrt{\mu_0/\varepsilon_0}$ is the impedance of free space; $\Delta S = L_x L_y$ is the area of the unit cell of the metamaterial; $L_x$ and $L_y$ are recurrence intervals of meta-atoms in the metamaterial along the $x$ and $y$ axes.

The expressions for the scattered field produced by a plane grating composed of electric quadrupole and magnetic dipole moments are found in a similar way:

$$\boldsymbol{E}_{\mathrm{sc}}^{\mathrm{qm}} = -\frac{1}{2\varepsilon_0 k_{0z}\Delta S}\exp[\mathrm{i}(\boldsymbol{k}_0'\boldsymbol{r})][\boldsymbol{k}_0'[\boldsymbol{k}_0'(\hat{\boldsymbol{M}}\boldsymbol{k}_0')]],$$

$$\boldsymbol{H}_{\mathrm{sc}}^{\mathrm{qm}} = \frac{1}{2\varepsilon_0 Z_0 k_0 k_{0z}\Delta S}\exp[\mathrm{i}(\boldsymbol{k}_0'\boldsymbol{r})][\boldsymbol{k}_0'[\boldsymbol{k}_0'[\boldsymbol{k}_0'(\hat{\boldsymbol{M}}\boldsymbol{k}_0')]]]. \quad (6)$$

In order to analyse the magnetic properties of metamaterials, it is important to separate the contributions of the electric quadrupole and magnetic dipole moments. This separation can be done if we take into account the fact that the combined tensor $\hat{\boldsymbol{M}}$ can be represented as the sum of symmetric and asymmetric parts, the symmetric part corresponding to the electric quadrupole moment, and antisymmetric – to the magnetic dipole moment [9]:

$$(\hat{\boldsymbol{M}}\boldsymbol{n})^{\mathrm{q}} = \frac{\varepsilon_0}{2}\int(\varepsilon(\boldsymbol{r}') - 1)(\boldsymbol{E}(\boldsymbol{n}\boldsymbol{r}') + \boldsymbol{r}'(\boldsymbol{E}\boldsymbol{n}))\mathrm{d}V',$$

$$(\hat{\boldsymbol{M}}\boldsymbol{n})^{\mathrm{m}} = \frac{\varepsilon_0}{2}\int(\varepsilon(\boldsymbol{r}') - 1)[[\boldsymbol{r}'\times\boldsymbol{E}]\times\boldsymbol{n}]\mathrm{d}V', \quad (7)$$

where $(\hat{\boldsymbol{M}}\boldsymbol{n})^{\mathrm{q}}$ is the projection vector of the electric quadrupole moment of the particle, and $(\hat{\boldsymbol{M}}\boldsymbol{n})^{\mathrm{m}}$ is the projection vector of the magnetic dipole moment of the particle in the direction $\boldsymbol{n}$.

Now, the electric and magnetic fields from an infinite plane of particles taking into account only the electric quadrupole moment will have the form:

$$\boldsymbol{E}_{\rm sc}^{\rm q} = -\frac{1}{2\varepsilon_0 k_{0z}\Delta S}\exp[{\rm i}(\boldsymbol{k}_0'\boldsymbol{r})][\boldsymbol{k}_0'[\boldsymbol{k}_0'(\hat{\boldsymbol{M}}\boldsymbol{k}_0')^{\rm q}]],$$

$$\boldsymbol{H}_{\rm sc}^{\rm q} = \frac{1}{2\varepsilon_0 Z_0 k_0 k_{0z}\Delta S}\exp[{\rm i}(\boldsymbol{k}_0'\boldsymbol{r})][\boldsymbol{k}_0'[\boldsymbol{k}_0'[\boldsymbol{k}_0'(\hat{\boldsymbol{M}}\boldsymbol{k}_0')^{\rm q}]]], \quad (8)$$

$$(\hat{\boldsymbol{M}}\boldsymbol{k})^{\rm q} = \frac{\varepsilon_0}{2}\int(\varepsilon(\boldsymbol{r}') - 1)(\boldsymbol{E}(\boldsymbol{r}')\boldsymbol{k}_0' + \boldsymbol{r}'(\boldsymbol{E}(\boldsymbol{r}'))\boldsymbol{k}_0'))\,{\rm d}V'.$$

Then, the contribution to the scattered field from the magnetic dipoles can be written as

$$\boldsymbol{E}_{\rm sc}^{\rm m} = \boldsymbol{E}_{\rm sc}^{\rm qm} - \boldsymbol{E}_{\rm sc}^{\rm q},\ \boldsymbol{H}_{\rm sc}^{\rm m} = \boldsymbol{H}_{\rm sc}^{\rm qm} - \boldsymbol{H}_{\rm sc}^{\rm q}. \quad (9)$$

Since the field inside the nanoparticles that make up the metamaterial are found using numerical simulations, formulas (5), (6) and (8) for the components of the scattered field, caused by various multipole moments, can be used to determine the characteristics of the far field. In particular, we can obtain the transmission, reflection and absorption coefficients, calculate the Stokes parameters of the transmitted and reflected waves, to determine their polarisation, and to calculate the effective parameters $\varepsilon_{\rm eff}$ and $\mu_{\rm eff}$ of the medium made of this metamaterial [10, 11].

To derive the specific expressions for the transmission coefficient, it is needed to calculate the flux of the electromagnetic energy transmitted through the metamaterial layer, i.e., Umov–Poynting vector for the sum of the external (incident on the particles) field and the scattered field, and then to divide its $z$-component by the $z$-component of the Umov–Poynting vector of the external field. The total (electric and magnetic) field in the transmitted wave is given by the expression

$$\boldsymbol{E}_{\rm T} = \boldsymbol{E}_{\rm sc}^{\rm d} + \boldsymbol{E}_{\rm sc}^{\rm qm} + \boldsymbol{E}_0,\ \boldsymbol{H}_{\rm T} = \boldsymbol{H}_{\rm sc}^{\rm d} + \boldsymbol{H}_{\rm sc}^{\rm qm} + \boldsymbol{H}_0, \quad (10)$$

where $\boldsymbol{E}_0(\boldsymbol{r}) = \boldsymbol{E}_0\exp[{\rm i}(\boldsymbol{k}_0\boldsymbol{r})]$, $\boldsymbol{H}_0(\boldsymbol{r}) = \boldsymbol{H}_0\exp[{\rm i}(\boldsymbol{k}_0\boldsymbol{r})]$, $|\boldsymbol{H}_0| = H_0 = Z_0^{-1}|\boldsymbol{E}_0| = Z_0^{-1}E_0$ are the external electric and magnetic fields; and $Z_0$ is the impedance of free space. The averaged Umov–Poynting vector of the transmitted wave takes the form

$$\boldsymbol{S}_{\rm T} = \frac{1}{2}{\rm Re}[\boldsymbol{E}_{\rm T}\times\boldsymbol{H}_{\rm T}^*] = \frac{1}{2Z_0}{\rm Re}\Big[E_0^2 + \frac{1}{\varepsilon_0 k_{0z}\Delta S}(\boldsymbol{E}_0\boldsymbol{P}_{\rm qm})$$

$$+ \frac{1}{(2\varepsilon_0 k_{0z}\Delta S)^2}(|\boldsymbol{P}_{\rm d}|^2 + |\boldsymbol{P}_{\rm qm}|^2)\Big]\frac{\boldsymbol{k}_0^{\rm T}}{k_0}, \quad (11)$$

where

$$\boldsymbol{P}_{\rm d} = [\boldsymbol{k}_0^{\rm T}[\boldsymbol{k}_0^{\rm T}\boldsymbol{d}]], \quad \boldsymbol{P}_{\rm qm} = [\boldsymbol{k}_0^{\rm T}[\boldsymbol{k}_0^{\rm T}(\hat{\boldsymbol{M}}\boldsymbol{k}_0^{\rm T})]]. \quad (12)$$

The averaged Umov–Poynting vector of the incident wave has the form

$$\boldsymbol{S}_0 = \frac{1}{2}{\rm Re}[\boldsymbol{E}_0\times\boldsymbol{H}_0^*] = \frac{1}{2Z_0}E_0^2\frac{\boldsymbol{k}_0}{k_0}.$$

As a result, the transmission coefficient is expressed through the multipole moments of the meta-atom:

$$T = \frac{S_{{\rm T}z}}{S_{0z}} = 1 + \frac{1}{E_0^2}{\rm Re}\Big[\frac{1}{\varepsilon_0 k_{0z}\Delta S}(\boldsymbol{E}_0\boldsymbol{P}_{\rm qm})$$

$$+ \frac{1}{(2\varepsilon_0 k_{0z}\Delta S)^2}(|\boldsymbol{P}_{\rm d}|^2 + |\boldsymbol{P}_{\rm qm}|^2)\Big]. \quad (13)$$

The reflection coefficient is calculated similarly, with the only difference being that the $z$-component of the Umov–Poynting vector of the reflected field is normalised to the same component of the incident field. The reflected fields have the form:

$$\boldsymbol{E}_{\rm R} = \boldsymbol{E}_{\rm sc}^{\rm d} + \boldsymbol{E}_{\rm sc}^{\rm qm},\ \boldsymbol{H}_{\rm R} = \boldsymbol{H}_{\rm sc}^{\rm d} + \boldsymbol{H}_{\rm sc}^{\rm qm}. \quad (14)$$

Then, the reflection coefficient is

$$R = \frac{1}{E_0^2}\frac{1}{(2\varepsilon_0 k_{0z}\Delta S)^2}{\rm Re}(|\boldsymbol{P}_{\rm d}|^2 + |\boldsymbol{P}_{\rm qm}|^2), \quad (15)$$

where

$$\boldsymbol{P}_{\rm d} = [\boldsymbol{k}_0^{\rm R}[\boldsymbol{k}_0^{\rm R}\boldsymbol{d}]]; \quad \boldsymbol{P}_{\rm qm} = [\boldsymbol{k}_0^{\rm R}[\boldsymbol{k}_0^{\rm R}(\hat{\boldsymbol{M}}\boldsymbol{k}_0^{\rm R})]]. \quad (16)$$

Similarly, we can find other characteristics of the far fields, including the Stokes parameters and the effective values of the electric ($\varepsilon_{\rm eff}$) and magnetic ($\mu_{\rm eff}$) permeabilities.

Indeed, the constitutive equations for the quadrupole medium have the form [11]

$$\boldsymbol{D} = \varepsilon_0\boldsymbol{E} + \boldsymbol{P} - [\nabla\hat{\boldsymbol{Q}}] = \varepsilon\varepsilon_0\boldsymbol{E} + {\rm i}\chi\boldsymbol{H},$$

$$\frac{1}{\mu_0}\boldsymbol{B} = \boldsymbol{H} + \boldsymbol{M} = \mu\boldsymbol{H} - {\rm i}\chi\mathbf{E}, \quad (17)$$

where $\boldsymbol{P}$ is the electric polarisation vector; $\hat{\boldsymbol{Q}}$ is the tensor of the electric quadrupole moment per unit volume of the medium; and $\boldsymbol{M}$ is the magnetisation vector. These parameters are proportional to those found earlier for electric dipole, electric quadrupole and magnetic dipole moments of meta-atoms, respectively. They can also be expressed through periodicity cell averaged electric and magnetic fields in metamaterials:

$$M_\alpha = \chi_{\alpha\beta}^{(0)}H_\beta + \chi_{\alpha\beta\gamma}^{(1)}\nabla_\gamma H_\beta,$$

$$P_\alpha = p_{\alpha\beta}^{(0)}E_\beta + p_{\alpha\beta\gamma}^{(1)}\nabla_\gamma E_\beta, \quad (18)$$

$$Q_{\alpha\gamma} = q_{\alpha\gamma\beta}^{(0)}E_\beta + q_{\alpha\gamma\beta\delta}^{(1)}\nabla_\delta E_\beta,$$

where the tensors $p_{\alpha\beta}^{(0)}$ and $\chi_{\alpha\beta}^{(0)}$ contribute to the electric and magnetic permeabilities, respectively; and $p_{\alpha\beta\gamma}^{(1)}$, $\chi_{\alpha\beta\gamma}^{(1)}$ and $q_{\alpha\beta\gamma}^{(0)}$

are responsible for the chirality of the medium. Thus, using constitutive equations (17) and (18) we can obtain expressions for the effective electric and magnetic permeabilities, as well as for the chirality of the metamaterial. Note that to determine all the coefficients in (18), we need to use additional information (about the symmetry of the system and different angles of incidence and polarisation).

## 3. Illustration of the method effectiveness by the example of the metamaterial of H-shaped nanoparticles

To illustrate the use of the above approach, we simulated numerically and analysed the optical and polarisation properties of a planar metamaterial with H-shaped meta-atoms (Fig. 2). Meta-atoms of this material are complex enough to serve as a representative example of the use of our method. The nanoparticles were produced of gold (dielectric permittivity $\varepsilon$ is taken from [12], $\mu = 1$). Numerical simulation was carried out in COMSOL Multiphysics software environment. The incident field propagated along the normal to the surface of the metamaterial. The modelling was performed for two linear polarisations of the incident wave – for the electric field polarised along the $x$ and $y$ axes. The resulting calculations of the field were then exported to the Matlab package, where they were further processed. In particular, combining the results obtained for the different linear polarisations of the incident field, we calculated the metamaterial response to a wave with circular polarisation.

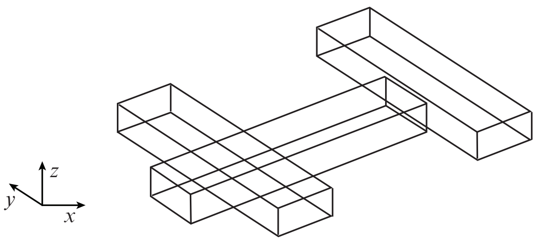


**Figure 2.** Structure of meta-atoms of which the metamaterial is assembled (see Fig. 1). Dimensions of the upper bar are 55×80×40 nm, the dimensions of the lower bars are 315×80×40 nm, the displacement of the upper bar with respect to the middle of the lower bars (along the $y$ axis) is 70 nm.

To check the accuracy of the approach in question, we compared the transmission and reflection coefficients calculated using COMSOL software and obtained by the proposed method. In COMSOL the transmission and reflection coefficients are calculated by averaging the Umov–Poynting vector in the $xy$ plane at $z = 250$ nm (behind the nanoparticle the total field is taken into account) and $z = -250$ nm (in front of the nanoparticles only the scattered field is taken into account), respectively. As can be seen from Fig. 3, the values of the coefficients coincide with a high degree of accuracy, which indicates the adequacy of the description of the interaction of light with a metamaterial with the help of the model of multipole moments. Generally speaking, in this paper we neglect the toroidal moment, which can make a significant contribution to the scattered field at other geometries of a meta-atom [13], but it can be easily taken into account within the framework of our approach.

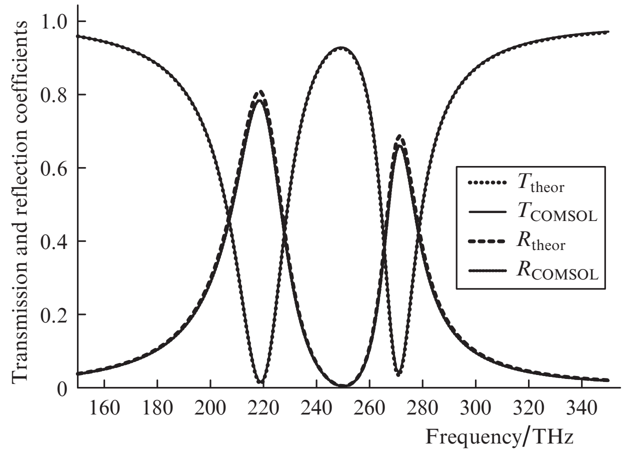


**Figure 3.** Transmission ($T_{theor}$) and reflection ($R_{theor}$) coefficients calculated by the multipole moments and the simulation software package ($T_{COMSOL}$ and $R_{COMSOL}$, respectively).

Of considerable interest is to study the contribution of different multipole moments separately, since it allows one to understand at a qualitative level the nature of this or that optical resonance. For greater clarity, we consider the contributions of different multipoles into transmission coefficients (Fig. 4). It can be seen that although the electric dipole contribution is dominant, it alone cannot accurately describe the response of the metamaterial to the incident field. Magnetic dipole and electric quadrupole moments have a significant impact on the position of the resonances and the magnitude of the transmission coefficient outside the resonances. Thus, although the electric dipole moment qualitatively determines the response of the metamaterial to the incident field, of importance for the exact numerical result is the contribution of higher multipole moments.

One more interesting result can be obtained from Fig. 4: despite the fact that the nanoparticles of the metamaterial are composed of a substance with $\mu = 1$, the magnetic response of the metamaterial is nonzero. Therein lies the fundamental dif-

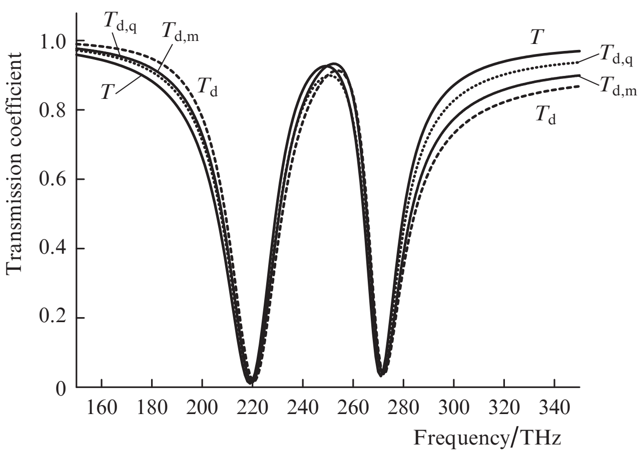


**Figure 4.** Transmission coefficients, taking into account the contributions of various multipole moments: ($T$) all the contributions are taken into account, ($T_d$) only the electric dipole moment is taken into account, ($T_{d,q}$) the electric dipole and quadrupole moments are taken into account, ($T_{d,m}$) the dipole electric and magnetic moments are taken into account. The incident wave is polarised along $x$.

ference of the metamaterial from the conventional macroscopic material: a metamaterial interacting with light exhibits unusual properties that cannot be observed in ordinary matter. Although the contribution of the magnetic dipole moment is small, it is essential that it is different from zero. This suggests the possibility of producing such a configuration of a nanoparticle in which its magnetic moment would be comparable in order of magnitude (or more) with an electric dipole moment and will make a significant contribution to the interaction of light with such a metamaterial.

As noted above, simulation using the COMSOL software package was conducted for two linear polarisations of the incident wave – along the $x$ axis and along the $y$ axis. Combining the solutions obtained for these linear polarisations, we can obtain any solution for the other polarisations, including circular. Thus, if we consider the wave propagating from the source, the fields with the right- and left-hand circular polarisations will be determined as:

$$\boldsymbol{E}_{\rm right}(\boldsymbol{r}) = \boldsymbol{E}_x(\boldsymbol{r}) + {\rm i}\boldsymbol{E}_y(\boldsymbol{r}), \qquad \boldsymbol{E}_{\rm left}(\boldsymbol{r}) = \boldsymbol{E}_x(\boldsymbol{r}) - {\rm i}\boldsymbol{E}_y(\boldsymbol{r}), \qquad (19)$$

where $\boldsymbol{E}_x(\boldsymbol{r})$ and $\boldsymbol{E}_y(\boldsymbol{r})$ are the solutions for linear $x$- and $y$-polarisations. Substituting the obtained solution into the expressions for the Stokes parameters, we can obtain the conversion coefficients of the wave with one circularly polarisation into the wave with the opposite circular polarisation. Since in this case the shape of the metamaterial nanoparticles is symmetric with respect to the left- and right-hand circular polarisations (i.e., the particle is not chiral), it is sufficient to obtain the results for the wave (passing through a layer of the metamaterial) of only one circular polarisation – for the opposite circular polarisation the result will be the same.

Consider the right-hand polarised wave incident on the metamaterial and its conversion. Figure 5 presents the amplitudes of the right- and left-hand polarised waves after passing through the metamaterial layer, normalised to their sum. One can see that in the region of resonances the transmitted wave is no longer a purely right-hand polarised wave, and near 275 THz, it has left-hand elliptical polarisation. At the points where the amplitudes of the right- and left-hand polarised waves intersect, the transmitted wave is linearly polarised. Figure 6 shows the amplitudes of the right- and left-hand polarised waves, normalised to transmission coefficient at the corresponding frequency. It can be seen that although about 60% of the transmitted right-hand polarised wave is converted into the left-hand polarised wave, with respect to the incident wave amplitude the conversion coefficient is much smaller – about 20%.

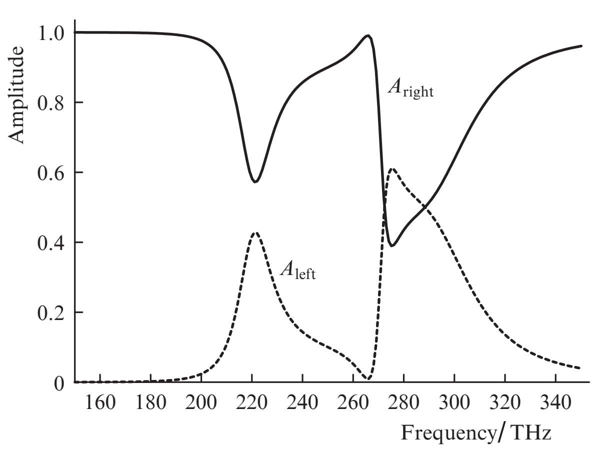


**Figure 5.** Amplitudes of the right- and left-hand circularly polarised waves passing through the layer of the metamaterial. The amplitudes are normalised to their sum; the right-hand circularly polarised wave is incident on the metamaterial.

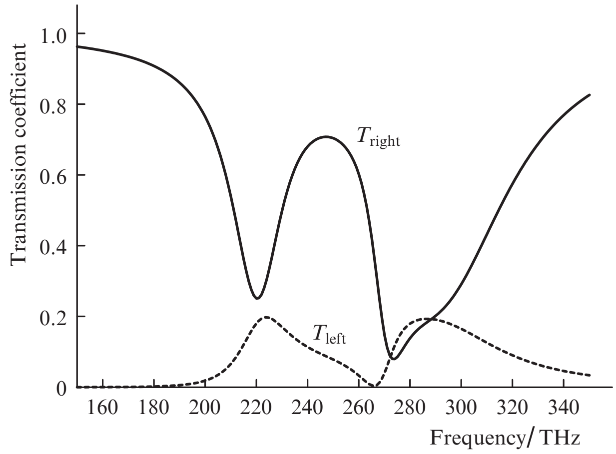


**Figure 6.** Amplitudes of the right- and left-hand circularly polarised waves passing through the layer of the metamaterial. The amplitudes are normalised to the transmission coefficient; the right-hand circularly polarised wave is incident on the metamaterial.

As in the case of linear polarisation, we compare the contributions of the various multipole moments into the transmission coefficient. Figure 7 shows the spectra of the transmission coefficient taking into account different combinations of multipole moments. One can see that dominant is the electric dipole moment; however, the corresponding transmission coefficient is significantly different from the total transmission coefficient taking into account all the three contributions in the case of linear polarisation. In this case, the account for the dipole electric moment with the magnetic dipole moment almost does not change the situation, whereas the account for the dipole electric moment with the electric quadrupole moment significantly improves the coincidence with

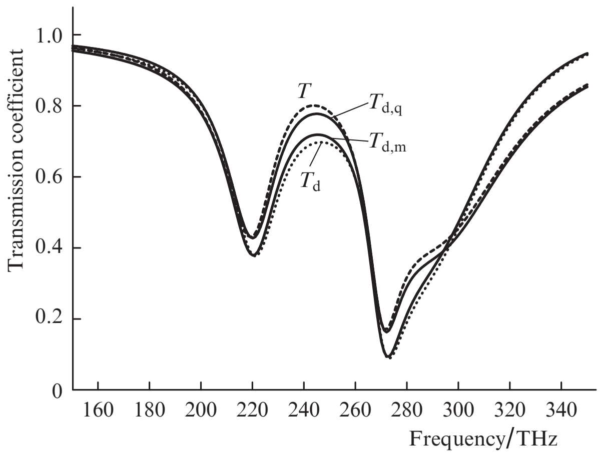


**Figure 7.** Transmission coefficients, taking into account the contributions of various multipole moments (notation is the same as in Fig. 4). The right-hand circularly polarised wave is incident on the metamaterial.

the total transmission coefficient. From this we can conclude that when a circularly polarised wave interacts with the metamaterial nanoparticles, the contribution of the quadrupole electric moment is much greater than that of the magnetic dipole moment.

## 4. Conclusions

We have developed a new method for determining the optical properties of planar metamaterials based on the calculation of multipole moments of meta-atoms which, when applied to the results of numerical simulation of interaction of light with a planar metamaterial, allows one to study its optical and polarisation properties. As an example of this method, we have investigated the metamaterial with meta-atoms in the form of H-shaped nanoparticles. We have calculated the multipole moments induced by the incident field in the nanoparticles, and then the results have been used to calculate the transmission and reflection coefficients, the far field and the Stokes parameters. By combining the numerical results obtained for the two linear polarisations of the incident wave, we have constructed a solution for the circular polarisation of the incident wave, and studied the properties of the metamaterial for this case. In particular it has been shown that the metamaterial in question in some frequency range converts the incident circularly polarised wave into the elliptically polarised wave and other direction of rotation. The results obtained show that the proposed method is very accurate and can be used in the analysis of arbitrary metamaterials.

This paper does not take into account the toroidal moments [13] induced in the nanoparticles (the influence of these moments in our case is negligible). When they are taken into account, it is possible to further expand the method of multipole moments. In addition, the method of multipole moments allows one to calculate the effective parameters $\varepsilon$ and $\mu$ of the medium, and therefore can be used as an alternative to the method proposed in [10], which is, however, beyond the scope of the research presented in this paper.

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