The numerical simulation and investigation of plasmonic properties of clusters consisted of two nanoparticles

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Abstract. Resonant properties of subwavelength spherical particles in strongly anisotropic metamaterials were investigated in this paper by means of spherical harmonics expansion. Numerical simulation of such problem using finite element method was demonstrated in COMSOL Multiphysics software.

1. Introduction
In the recent years scientists are occupied with studying of metamaterials (MM). There are artificially created materials that can realize some interesting effects at any frequency [1-3]. Different devices components can be created from MM [4,5]. There are some approaches for studying different MM [6]. Now the nanoplasmonics is topical because of one can see localization and amplification of the optical field (luminous edge effect) due to the substance in a nanoscale space. On the other side metal particles have eigen modes on frequencies ranged from ultraviolet to infrared wavelength range. Both of these peculiarities determine an attractive and complicated physics one observes, that serves as a basis for many applications [7-9]. Clusters containing several nanoparticles (so-called determinate structures or nanoparticle arrays/gratings) are of special interest to scientists by the side of the single (isolated) plasmonic nanoparticles [10] which properties are particularly interesting and have a number of significant applications. This interest is caused by that clusters unlike single nanoparticles have at least two various parameters: the size of nanoparticles and the distance between them. If we vary any of these parameters plasmonic properties of nanoparticles will essentially change, that enables us to exercise significant influence over them and spectrum of plasmon-polariton oscillations, to ensure coupling between clusters containing plasmonic nanoparticles with atoms, molecules and other nanoscale devices. Such versatility affords an opportunity to create the most diverse nanostructures [11-14]. Furthermore, there are strong local fields in the clearance between nanoparticles that can be several orders greater than incident fields and be required for a plenty of applications as well. The most fundamental significance has clusters containing two subwavelength particles, which this paper is devoted to, namely clusters containing two subwavelength spherical one size particles. To be more exact, it is supposed to consider an anisotropy of both subwavelength spherical particles and the medium apart from the already studied isotropic nanoparticles in the optically isotropic medium. Investigation of the nature of nontrivial eigen resonances and their impact on the local field correction for emission processes in THz frequency range will be studied here.
2. Quasistatic Model for two couple spherical particles inside anisotropic uniaxial medium

Plasmon modes of cluster located in the anisotropic medium and containing two subwavelength particles can be found by means of «ε-method» as well as in case of cluster located in the dielectric (isotropic) background.

It demands a solution of eigen modes of the system in the quasistatic limit by adopting Laplace equation for electric potential with continuity of it and the normal component of the displacement at the boundary:

\[ E = -\nabla \varphi, \quad \text{div}(\varepsilon \text{grad} \varphi) = 0, \]
\[ [\varphi]_S = 0, \quad \left[ \frac{\varepsilon \varphi}{\frac{\partial \varphi}{\partial n}} \right]_S = 0, \]

where \( \varepsilon \) represented by eq. 2 (\( \varepsilon_{\text{out}} \) is \( \varepsilon \) outside the particle, \( \varepsilon_{\text{in}} \) is \( \varepsilon \) inside the particle).

\[ \varepsilon = \begin{cases} \varepsilon_{\text{out}} = \text{diag}(\varepsilon_1, \varepsilon_2, \varepsilon_3) \\ \varepsilon_{\text{in}} \end{cases}. \]

The equation \( \text{div}(\varepsilon \text{grad} \varphi) = 0 \) in (1) for the eigen modes determination problem for two subwavelength particles located in the anisotropic medium disintegrates into system of two equations, for the potential inside and outside the particles (spheres) respectively:

\[ \begin{cases} \frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2} = 0, & \text{inside the particles.} \\ \varepsilon_1 \frac{\partial^2 \varphi}{\partial x^2} + \varepsilon_2 \frac{\partial^2 \varphi}{\partial y^2} + \varepsilon_3 \frac{\partial^2 \varphi}{\partial z^2} = 0, & \text{outside the particles.} \end{cases} \]

It will be more convenient to solve this problem in bispherical coordinates which are obtained by rotating a two-dimensional bipolar coordinate system about the axis connecting its two poles. Coordinates in such system \((-\infty < \eta < \infty, \ 0 < \xi \leq \pi, \ 0 \leq \phi < 2\pi)\) and the Cartesian coordinates are related as follows:

\[ x = a \frac{\sin \xi \cos \phi}{\cosh \eta - \cos \xi}, \quad y = a \frac{\sin \xi \sin \phi}{\cosh \eta - \cos \xi}, \quad z = a \frac{\sinh \eta}{\cosh \eta - \cos \xi}. \]

Lamé coefficients of such coordinate system are:

\[ h_\xi = h_\eta = \frac{a}{\cosh \eta - \cos \xi}, \quad h_\phi = \frac{a \sin \xi}{\cosh \eta - \cos \xi}. \]

The first equation of the system (3) in bispherical coordinates converts into the following equation:

\[ \Delta \varphi = \frac{1}{h_\xi^2} \left[ \frac{\partial}{\partial \xi} \left( h_\eta \frac{\partial \varphi}{\partial \eta} \right) + \frac{1}{\sin \xi} \frac{\partial}{\partial \xi} \left( h_\eta \sin \xi \frac{\partial \varphi}{\partial \xi} \right) + \frac{h_\eta}{\sin^2 \xi} \frac{\partial^2 \varphi}{\partial \phi^2} \right] = 0. \]

The solution of this equation is well-known [15, 16]. Variables in the Laplace’s equation (6) can be separated only after the substitution \( \varphi = \sqrt{\cosh \eta - \cos \xi} \ F, \) where \( F = M(\eta)N(\xi)\Phi(\phi) \). Then, the equation (6) transforms into equation (7):

\[ \frac{\partial^2 F}{\partial \eta^2} + \frac{1}{\sin \xi} \frac{\partial}{\partial \xi} \left( \sin \xi \frac{\partial F}{\partial \xi} \right) + \frac{1}{\sin^2 \xi} \frac{\partial^2 F}{\partial \phi^2} - \frac{1}{4} F = 0. \]

The anisotropy \( \varepsilon_{\text{out}} \) represented by the tensor \( \text{diag}(\varepsilon_1, \varepsilon_2, \varepsilon_3) \) complicates the solution of the second equation of the system (3). The above-mentioned tensor in bispherical coordinates converts into the following:
The presumption \( \varepsilon_1 = \varepsilon_2 = \varepsilon \) was made to simplify the problem. The distribution of normalized electric field was simulated at the terahertz frequency range by the means of the Radio Frequency module of the COMSOL Multiphysics software, see Fig. 1.

3. Numerical simulation results

Figure 1 (a) shows simulation of the distribution of normalized electric field component of two subwavelength particles isotropic background at the frequency of 1.0009 THz with the following parameters: the radius of the particles \( R=0.5 \) mm, the distance between the particles \( R_{12}=1.17 \) mm, the permittivity of the particles \( \varepsilon_{in} = 1 \), the permittivity of the dielectric (isotropic) background \( \varepsilon_{out} = -0.5 \). In Figure 1 (b) it is demonstrated the simulation of the distribution of normalized electric field component of two subwavelength particles anisotropic background at the frequency of 1.0031 THz with the radius of the particles \( R=0.5 \) mm, the distance between the particles \( R_{12}=1.17 \) mm, the permittivity of the particles \( \varepsilon_{in} = 1 \), the permittivity of the anisotropic background \( \tilde{\varepsilon}_{out} = \text{diag}(0.5,0.5,-1.5) \).

![Figure 1](image)

Figure 1. Distribution of normalized electric field component in the cluster containing two subwavelength particles: (a) dielectric (isotropic) background, (b) anisotropic background.

4. Conclusions

In this paper resonant properties of two subwavelength particles in anisotropic metamaterials by means of spherical harmonics expansion were investigated. These harmonics are nontrivially coupled by strong anisotropy and corresponding boundary conditions. The permittivity tensor in bispherical coordinates for anisotropic background was found. The electric field inside and outside particles was considered by means of spherical harmonics expansion. The field distribution simulation for the cluster containing two subwavelength particles and located in both anisotropic and isotropic background was performed by the means of the COMSOL Multiphysics software.

Acknowledgement

This work was financially supported by Government of Russian Federation, Grant 074-U01.

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