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Analysis of the use of the LCR circuit model for evaluating the resonant response of thin rectangular nanoantennas

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Abstract. **We demonstrate the possibility of estimating in a simple way the expected frequency of the resonant response to an external electromagnetic field in a thin golden nanoantenna having a rectangular cross section. The paper considers nanoantennas with a thickness smaller than the thickness of the skin layer or comparable with it. Analytical expressions for estimating the resonance response are presented, and full-wave simulation is performed. The algorithm for obtaining such estimates is important, in particular, for planning experiments without using full-wave simulation, which is often rather resource consuming. To obtain analytical expressions, a refined LCR circuit model is used. The analytical estimates obtained for the characteristics of the resonant response are in good agreement with the results of the full-wave simulation.**

Keywords: *nanoantennas, nanobar, broadband resonance, resonant response, LCR circuit model.*

1. Introduction

The resonant frequency response of metallic and dielectric micro- and nanoparticles is known to be determined by the material, characteristic dimensions, and geometry of such a particle. In this paper, we consider metal particles with a resonant response in the visible and near-IR regions. As a response, both absorption and scattering of light can be considered. Important characteristics of any resonance are the resonant frequency and quality factor (the reciprocal of the resonance relative width). In a number of practical applications, the broadband response of nanoparticles is of interest, i. e., a resonance with a large width and a low Q-factor. These are, for example, problems of broadband filtering in telecommunication technologies and tasks of sensorics, in which complex absorption spectra are recorded against the background of a broad plasmon resonance. Research in the field of producing a broadband response is being conducted intensively; in particular, several interesting works have recently been published, focused on developing a concept (geometry) for obtaining a broadband response for various technological applications, such as a polarisation converter, a broadband absorber, and control of chromatic aberrations [1–4].

As is known, plasmon resonances are inherently broad ones; therefore, in this paper we explore the possibilities of constructing an adequate assessment of plasmon resonances for nanoparticles having the shape of a nanobar with a rectangular cross section (Fig. 1). This shape is of interest due to the simplicity of the deposition of nanoparticles on a solid substrate, in particular, using the method of nanolithography in the course of manufacturing ordered meta-surfaces. This geometry of individual nanoblocks was used in Refs [1–4]. Note that if both sides of a rectangular section of a nanobar are sufficiently small (a wire), then for such particles the cross section shape is not important and there are other methods of approximation (cylinders of equivalent section [5]).

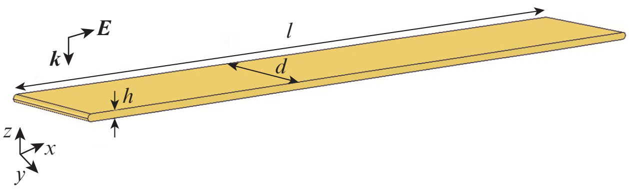

Figure 1. Golden nanoantenna (nanobar).

It should be noted that full-wave, especially three-dimensional, modelling of the resonant response of meta-surfaces requires large computational resources, and so it would be useful to be able to have plausible estimates for the resonance characteristics, such as resonance frequency and resonance width (Q-factor), i. e., a simple and adequate model. Such a model based on a quasi-static approximation for particles much smaller than the wavelength of the incident light was constructed in classical papers [6, 7], where simple analytical expressions for the nanoparticle response were derived. Particles of various geometry are analysed in detail, in particular, when a nanoparticle is a triaxial ellipsoid. In this paper, we do not limit ourselves to the quasi-static approximation and analyse the possibility of applying the LCR model of an oscillatory circuit [8, 9] for a more general case. In particular, as will be shown below, the use of the LCR circuit model makes it possible to obtain analytical evaluation formulas for the resonance frequency.

The advantages of this form of nanoantenna include the fact that, in the case of a rectangular antenna, there are three independent parameters for adjusting the resonant frequ-

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ency: length, width, and thickness. By fixing, for example, the length and width and varying the antenna thickness, we can adjust the resonant response frequency, in particular, as shown in Ref. [10], where the optical response of a cylindrical nanoantenna was studied depending on the form factor, which is the ratio of cylinder length to its diameter. A significant change in the response frequency depending on such a form factor was shown [10]. For the geometry considered in this work (Fig. 1), we can introduce two form factors: the ratio of length to thickness (l/h) and the ratio of length to width (l/d). Another independent coordinate appearing in the considered geometry provides an additional degree of freedom for the selection of the resonance width. In this paper, we study the normal incidence of an external electromagnetic field on a gold nanoantenna up to 20 nm thick, which corresponds to the upper limit of the skin layer for the IR spectrum. In the future, considering a rectangular nanoantenna, for brevity, we will call it a nanobar.

2. LCR-model as applied to micro-nanoparticles

In this paper, we intend to compare the results of a full-wave calculation of the characteristics of scattering of light by a gold nanobar and the estimate of the scattering parameter in a model where the nanobar is considered as an electrical circuit, namely, a series oscillatory circuit. For the first time, the idea of considering a nanoobject as an oscillatory circuit was proposed in Ref. [9] to describe the resonance scattering of light by a gold nanosphere. In addition, the use of this approach is described in Ref. [8].

In Ref. [11], a nanorod with circular cross section was considered as a light scatterer, the electric field strength vector being directed along the axis of the nanorod. A good agreement with the experimental results was obtained for the resonance wavelength of the scattered light in the LCR circuit model, but taking into account the adjustable multiplier and for the lengths corresponding to the quasi-static approximation. In the same paper, a simple analytical formula was proposed for the resonance wavelength by replacing the circular nanorod with a nanobar of rectangular cross section. The calculation using the formulas of Ref. [11] is in good agreement with the results of other works for a nanorod with circular cross section. However, as will be shown below, for nanobars, the results of such calculations are noticeably different from the results of full-wave calculations, especially for cases beyond the quasi-static model.

We decided to refine the corresponding formulas, remaining within the framework of the LCR circuit model, but not only within the quasi-static approximation, and obtain a simple analytical approximation for them. The main refinement is related to the mode composition of the resonances, which is particularly important beyond the quasi-static case. In the simplest model [11], it was assumed that at each instant of time the current density is the same at all points of the nanorod volume and is directed along its axis; in particular, it is the same along the entire length. However, as indicated by many authors, the current density at each time point is proportional to $\sin x$, where x is the coordinate along the axis of the nanorod (or nanobar). In particular, the possibility of a complex mode composition inside the nanoantenna is already apparent for particles that are much smaller than the wavelength. For the quasi-static case, a detailed full analysis is given for spheroidal particles in Ref. [6]. At the ends of the nanorod, the sinusoid should go to zero (for the dipole mode) in the case of a rectangular cross section. Accordingly, for the lower (dipole) mode, the half-wavelength of the sinusoid should be equal to the length of the nanorod. The authors of Ref. [10], in which the dipole mode for a circular-section nanorod is considered, have already made this refinement of the LCR model.

In Refs [10, 11] the authors considered the contribution to the loop inductance L_0, specific for nanosamples and related to the kinetic energy or momentum of the drift motion of electrons. With the increase in the nanosample size, this contribution becomes relatively small compared with the usual inductance. The value of L_0 is found by equating the kinetic energy of the electrons of the current to the inductance energy $L_0 I^2/2$, whence $L_0 = l m_e / S n_e e^2$ is obtained, where l and S are the length and cross-sectional area of the nanosample; m_e is the electron mass; n_e is the concentration of conduction electrons in gold; and e is the electron charge modulus. The value of the expression $n_e e^2/m_e$ can be obtained by relying on the well-known experiment value of the plasma frequency for gold $\omega_p = \sqrt{n_e e^2/m_e \varepsilon_0}$. Then

$$L_0 = \frac{l}{\varepsilon_0 \omega_p^2 S} = \frac{l\delta^2}{\varepsilon_0 c^2 S} = \frac{\mu_0 l \delta^2}{S}, \tag{1}$$

where ε_0 and μ_0 are the electric and magnetic constant, respectively, and the quantity $\delta = c/\omega_p = 21.9$ nm in accordance with Refs [10, 11] can be considered as the depth of penetration of the light field into gold. Note that for optical frequencies, the thickness of the skin layer of electric currents is several times smaller than this value.

In addition to the contribution L_0 to the inductance of an equivalent oscillatory circuit that is specific for nanosamples, there is also the traditional contribution L to the inductance. In Ref. [10], as in Ref. [11], it was proposed to find this contribution in accordance with the definition of inductance:

$$\frac{LI^2}{2} = \int_{V=\infty} \frac{\mu_0 H^2}{2} \mathrm{d}V. \tag{2}$$

In Ref. [10], it is proposed to find the capacitance of the oscillating circuit C in the same way:

$$\frac{Q^2}{2C} = \int_{V=\infty} \frac{\varepsilon_0 \varepsilon E^2}{2} \mathrm{d}V, \tag{3}$$

i.e., in a more correct way than in Ref. [11], where the capacitance is calculated between the ends of the cylinder using the approximation of a flat capacitor, followed by the introduction of a fitting coefficient of 2.5 to correct the resulting capacitance. In calculations using Eqn (3), the dielectric constant inside the nanoparticle is assumed equal to the dielectric constant of the environment of the nanoparticle basing on the fact that the volume of the nanoparticle is small and, therefore, contributes little to the integral. Plasmon losses are taken into account as losses on the ohmic resistance of the nanoparticle.

Fully agreeing with the formulas of Ref. [10] for calculating the capacitance and the traditional contribution to inductance, we note that integrals over an infinite volume can be replaced by integrals over the volume of a nanoobject, which greatly simplifies the calculations. Indeed, for example, the energy of the electric field can be found as the energy of the charges of the conductor:

$$\frac{Q^2}{2C} = \int_{V=\infty} \frac{\varepsilon_0 \varepsilon E^2}{2} \mathrm{d}V = \frac{1}{2}\int_{V_0} \rho\varphi \mathrm{d}V\,, \tag{4}$$

where V_0 is the volume of the nanosample; $\varepsilon = n^2$ is the dielectric constant of the medium surrounding the nanosample with a refractive index n; ρ is the bulk charge density; and

$$\varphi(\boldsymbol{r}) = \frac{1}{4\pi\varepsilon_0\varepsilon}\int_{V_0} \frac{\rho(\boldsymbol{r}')\mathrm{d}V'}{|\boldsymbol{r}-\boldsymbol{r}'|} \tag{5}$$

is the potential. With the mode composition of the resonances taken into account, the charge density is proportional to the cosine of the coordinate along the electric field $\boldsymbol{E}$ of the light wave. Hence, when the mode m is excited, we obtain for the capacitance of the nanoantenna:

$$C = \frac{2\varepsilon_0\varepsilon l}{\pi m^2 \displaystyle\int_{V_0}\int_{V_0'} \frac{\cos(m\pi x)\cos(m\pi x')}{|\boldsymbol{r}-\boldsymbol{r}'|}\mathrm{d}V'\mathrm{d}V}\,. \tag{6}$$

Here, l is the length of a nanobar or nanorod along the field $\boldsymbol{E}$; V_0 and V_0' is the same volume of the nanosample; x and x' is the coordinate inside the nanosample along the $\boldsymbol{E}$ field; and $\boldsymbol{r}$ and $\boldsymbol{r}'$ is the radius vector of the point inside the nanosample. The integrals are calculated in dimensionless variables, where each coordinate is scaled to the sample length l.

Similarly, the interaction energy of the currents can be related to the inductance:

$$\frac{LI^2}{2} = \int_{V=\infty} \frac{\mu_0 H^2}{2}\mathrm{d}V = \frac{1}{2}\int_{V_0} (\boldsymbol{jA})\mathrm{d}V\,, \tag{7}$$

$$\boldsymbol{A}(\boldsymbol{r}) = \frac{\mu_0}{4\pi}\int_{V_0} \frac{\boldsymbol{j}(\boldsymbol{r}')\mathrm{d}V'}{|\boldsymbol{r}-\boldsymbol{r}'|}\,, \tag{8}$$

$$L = \frac{\mu_0 l}{2\pi}\int_{V_0}\int_{V_0'} \frac{\sin(m\pi x)\sin(m\pi x')}{|\boldsymbol{r}-\boldsymbol{r}'|}\mathrm{d}V'\mathrm{d}V\,, \tag{9}$$

where $\boldsymbol{j}$ is the current density and the integral, as in Eqn (6), is taken over dimensionless variables scaled to the sample length l.

As a result, the resonant frequency of the mode with an arbitrary number m

$$\omega_m = \frac{1}{\sqrt{(L_0+L)C}} = \sqrt{\frac{\pi m^2 \displaystyle\int_{V_0}\int_{V_0'} \frac{\cos(\pi m x)\cos(\pi m x')}{|\boldsymbol{r}-\boldsymbol{r}'|}\mathrm{d}V'\mathrm{d}V}{2\varepsilon_0\varepsilon l\left(\dfrac{l}{\varepsilon_0\omega_\mathrm{p}^2 S} + \dfrac{\mu_0 l}{2\pi}\displaystyle\int_{V_0}\int_{V_0'} \frac{\sin(\pi m x)\sin(\pi m x')}{|\boldsymbol{r}-\boldsymbol{r}'|}\mathrm{d}V'\mathrm{d}V\right)}} \tag{10}$$

corresponds to the resonance wavelength $\lambda_\mathrm{res} = 2\pi c/\omega_\mathrm{res} = 2\pi c\sqrt{(L_0+L)C}$.

For a dipole mode ($m = 1$) using the least squares method, we found convenient approximating formulas for the integrals [in Eqns (6), (9) and (10)]:

$$J_{C1} = \int_{V_0}\int_{V_0'} \frac{\cos(\pi x)\cos(\pi x')}{|\boldsymbol{r}-\boldsymbol{r}'|}\mathrm{d}V'\mathrm{d}V \approx \ln\left(1 + \frac{0.382}{\left(\dfrac{hd}{l^2}\right)^{0.585}\left(\dfrac{d}{h}+\dfrac{h}{d}\right)^{0.345}}\right), \tag{11}$$

$$J_{L1} = \int_{V_0}\int_{V_0'} \frac{\sin(\pi x)\sin(\pi x')}{|\boldsymbol{r}-\boldsymbol{r}'|}\mathrm{d}V'\mathrm{d}V \approx \ln\left(1 + \frac{1.79}{\left(\dfrac{hd}{l^2}\right)^{0.515}\left(\dfrac{d}{h}+\dfrac{h}{d}\right)^{0.352}}\right). \tag{12}$$

Formulae (11) and (12) for approximating the integrals are valid with an accuracy of up to 5% for each of the pairs of values of the relative widths and thicknesses of the nanobar, shown in Fig.2.

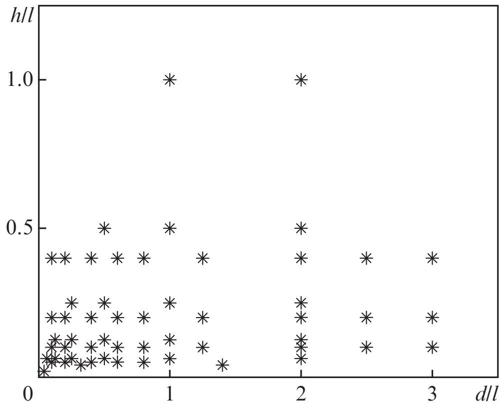

Figure 2. Range of variation of the inverse form factors of a nanobar, in which the approximations of the integrals for the inductance L and capacitance C using simple analytical formulas (11) and (12) are valid.

For the mode with the number m, the integrals change approximately like this:

$$J_{Cm} = J_{C1}\frac{a+1}{a+m} \;\text{ и }\; J_{Lm} = J_{L1}\frac{b+1}{b+m}\,,$$

where a and b are constants independent of m but dependent on the form factor of the nanobar. Substituting the obtained approximating formulas (11), (12) for integrals into the expression (10), we obtain an approximating formula for estimating the resonance frequency:

$$\omega_\mathrm{res} = \frac{1}{\sqrt{(L_0+L)C}} \approx \sqrt{\frac{\pi\ln\left(1 + \dfrac{0.382}{\left(\dfrac{hd}{l^2}\right)^{0.585}\left(\dfrac{d}{h}+\dfrac{h}{d}\right)^{0.345}}\right)}{2\varepsilon l^2\left[\dfrac{1}{\omega_\mathrm{p}^2 hd} + \dfrac{1}{2\pi c^2}\ln\left(1 + \dfrac{1.79}{\left(\dfrac{hd}{l^2}\right)^{0.515}\left(\dfrac{d}{h}+\dfrac{h}{d}\right)^{0.352}}\right)\right]}}\,. \tag{13}$$

3. Full-wave simulation of single nanoantennas with rectangular cross section

As mentioned above, the influence of one of the geometrical parameters, in particular diameter, on the position of the resonance response frequency of a cylindrical nanoantenna was studied in detail in Ref. [8]. The change in the response frequency as a function of the diameter (thickness) of such a cylindrical nanorods was found. In the present work, the resonance responses were studied when two parameters were changed (the width and thickness of the nanoantenna with a fixed length), whereas for a cylinder of circular cross section [8] the variable parameter was only the thickness (diameter). In this section, we present the results obtained by full-wave simulation for a nanobar of rectangular cross section. In the full-wave simulation, the Comsol Multiphysics (RF-module) package was used to solve the wave equation numerically, taking both the real and imaginary parts of the dielectric constant of the media into account. To simulate the field attenuation at infinity, the so-called perfectly matched PML layer was used. The numerical algorithm was implemented using the finite element grid method. As shown, e. g., in Ref. [12], at the moment such a numerical algorithm is the most reliable and approved one.

Nanobars with l = 100, 500 and 1000 nm were investigated. In this case, the thickness of the nanobars was chosen to be smaller than the thickness of the skin layer or of the order of it (h = 5, 10, 20 nm). This choice of thickness is caused by the fact that when deriving the approximate analytical expressions, by default it was assumed that there is a uniform current distribution across the thickness (along the z axis). The material of the simulated nanoantenna is gold. Experimentally obtained dispersion characteristics were used for computer calculations [13].

3.1. Numerical simulation for determining the resonance response of a nanobar

Figure 3 shows the spectral dependences of the scattering cross section for the gold nanoantenna with l = 500 nm and h = 5, 10, and 20 nm. The nanobar width d varied from 20 to 900 nm. The dependences have a resonance character with a resonance having the highest amplitude corresponding to the first dipole mode. As the width of the nanobar increases, the resonance wavelength decreases and the width of the resonance increases. At the left edge of the resonance, a feature is seen that can be identified as the third mode resonance. When the width of the nanobar changes, the resonances of the first and third modes move towards each other. With a normal incidence of light, the second mode is not excited.

It is clearly seen from Fig. 3 that in the selected frequency range the first dipole mode has a resonant response. It is also seen that with increasing nanobar width d, the resonance frequency increases (the resonance shifts shorter wavelengths) and becomes practically unchanging, when a certain width ($d \approx$ 800 nm) is exceeded. In addition, there is an expected increase in the width of the resonance curve with increasing h and d. Note that the behaviour of the width of the resonance curve requires a separate study and is not the primary task of

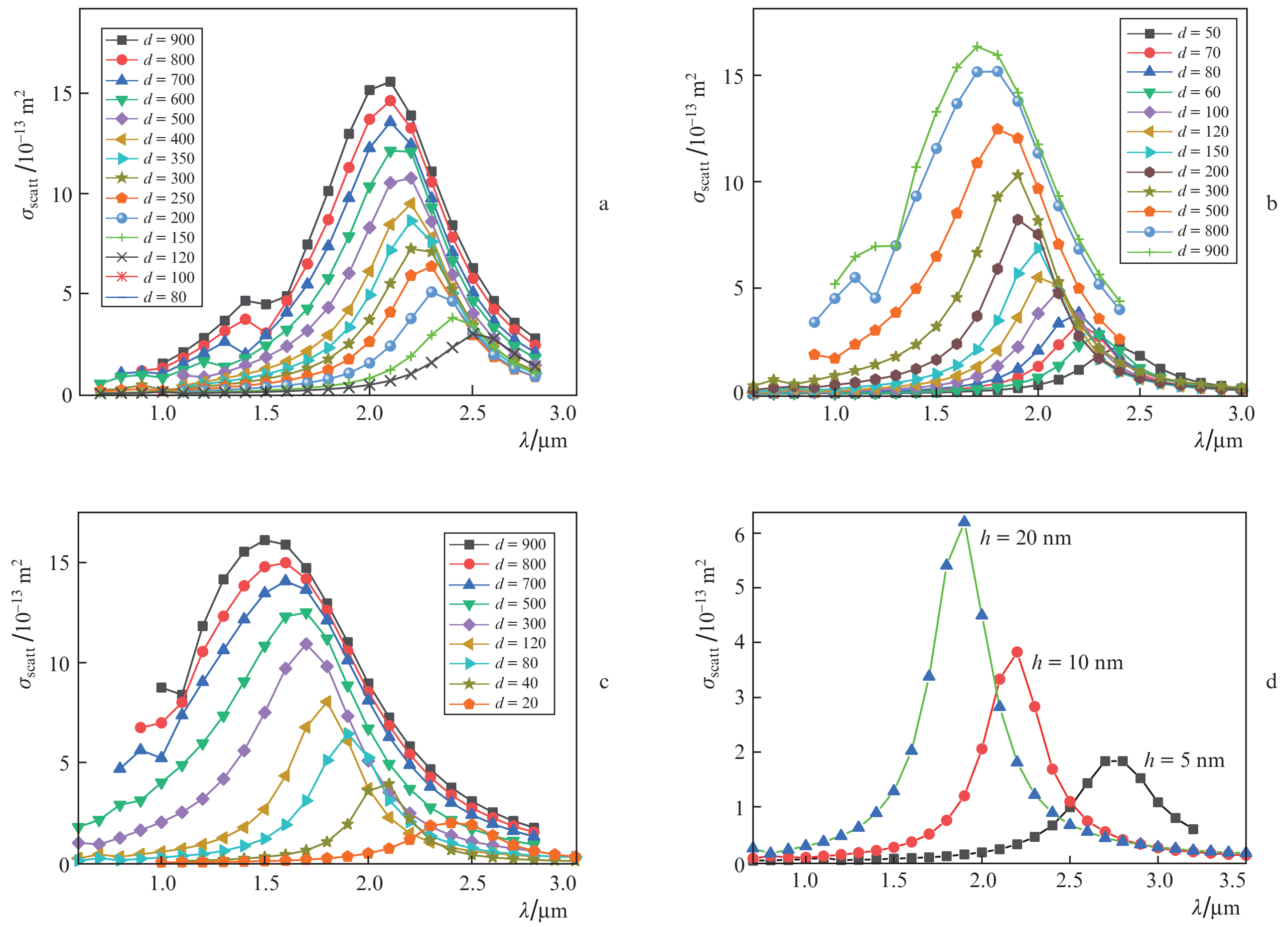

Figure 3. Scattering cross sections as functions of the wavelength of the incident radiation for l = 500 nm, different d and h = (a) 5, (b) 10, (c) 20 nm, and also for (d) d = 80 nm, l = 500 nm and h = 5, 10, 20 nm.

the present work. Figure 3d also shows the resonance responses for nanoantennas with l = 500 nm, d = 80 nm and various thicknesses. The presented dependences clearly demonstrate the relative shift of the frequency maxima and the corresponding increase in the amplitude of the scattering cross section with increasing nanoantenna thickness.

The behaviour of the frequency resonance response as a function of thickness coincides with the results of the calculations carried out by the authors of Ref. [14] for cylindrical nanoantennas of circular cross section.

In Fig. 4, for the golden nanoantenna with l = 1000 nm and h = 5 nm, the scattering cross section is shown as a function of wavelength for several values of d (from 80 to 500 nm). For an antenna with d = 500 nm, the third mode is quite clearly visible. For a nanobar with l = 100 nm, the character of the dependences of the scattering cross section is similar.

Figure 5 presents the calculated dependence of the scattering cross section for a nanoantenna with l = 1000 nm, h = 5 nm

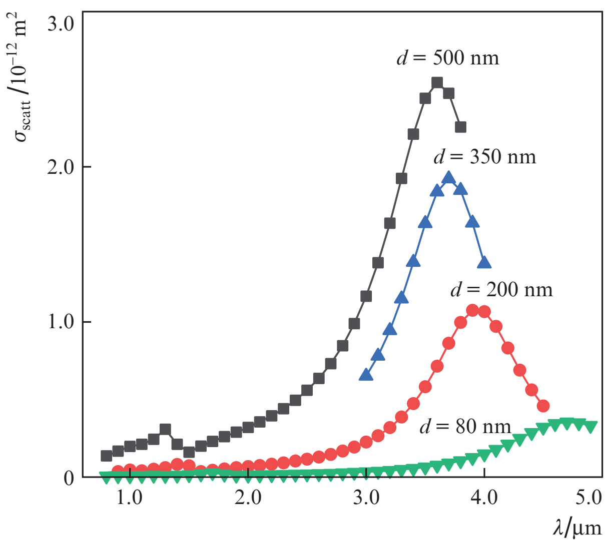

Figure 4. Dependence of the scattering cross section on the wavelength of the incident light for gold nanoantennas with l = 1000 nm, h = 5 nm, and different d.

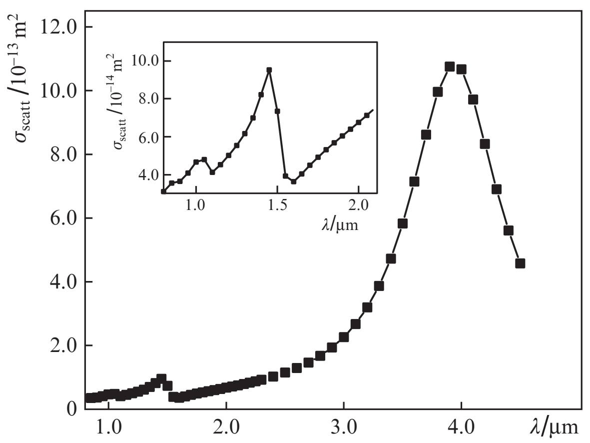

Figure 5. Calculated dependence of the scattering cross section for a nanoantenna with l = 1000 nm, h = 5 nm and d = 200 nm. The inset shows a fragment of this dependence in a magnified wavelength scale.

and d = 200 nm, for which relative magnitudes of the maxima for odd plasmon modes are clearly visible in a magnified wavelength scale.

Figure 6 shows the dependences of the resonance wavelength on the width d of nanobars with l = 100, 500 and 1000 nm and h = 5, 10, 20 nm. It can be seen that the resonance response has two characteristic regions: the nonlin-

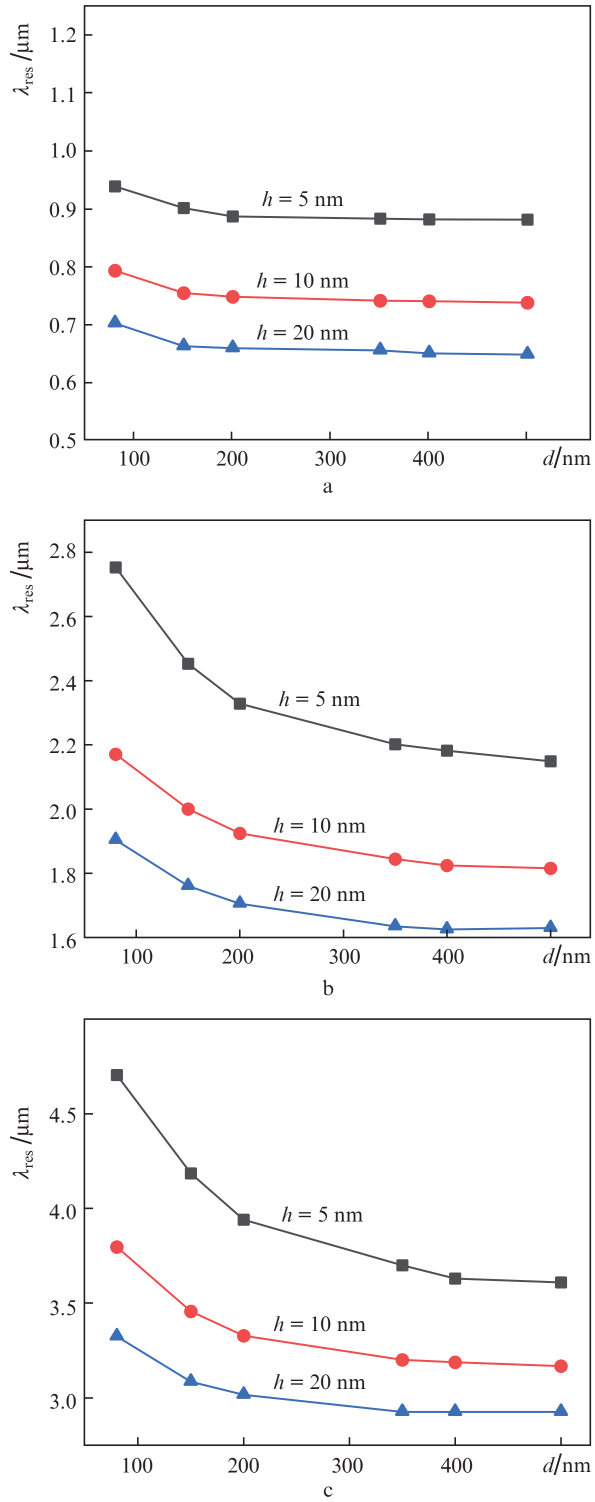

Figure 6. Dependences of the resonance wavelength on the widths d of nanobars with l = (a) 100, (b) 500, (c) 1000 nm and h = 5, 10, 20 nm.

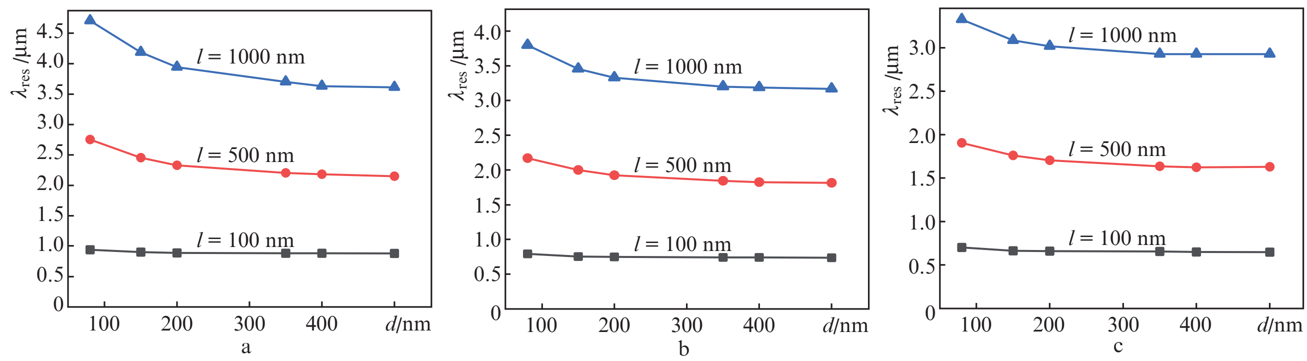

Figure 7. Dependences of the resonance wavelength on the width d of nanobars with h = (a) 5, (b) 10, (c) 20 nm and l = 100, 500, 1000 nm.

ear region of fast changing λ_{res} up to the width $d \approx 300$ nm and the linear region, where λ_{res} changes very slowly with increasing d.

Figure 7 shows the same dependences, but grouped for identical thicknesses h = (a) 5, (b) 10, (c) 20 nm. Here it can be clearly seen that in the range of rapid change of λ_{res} an

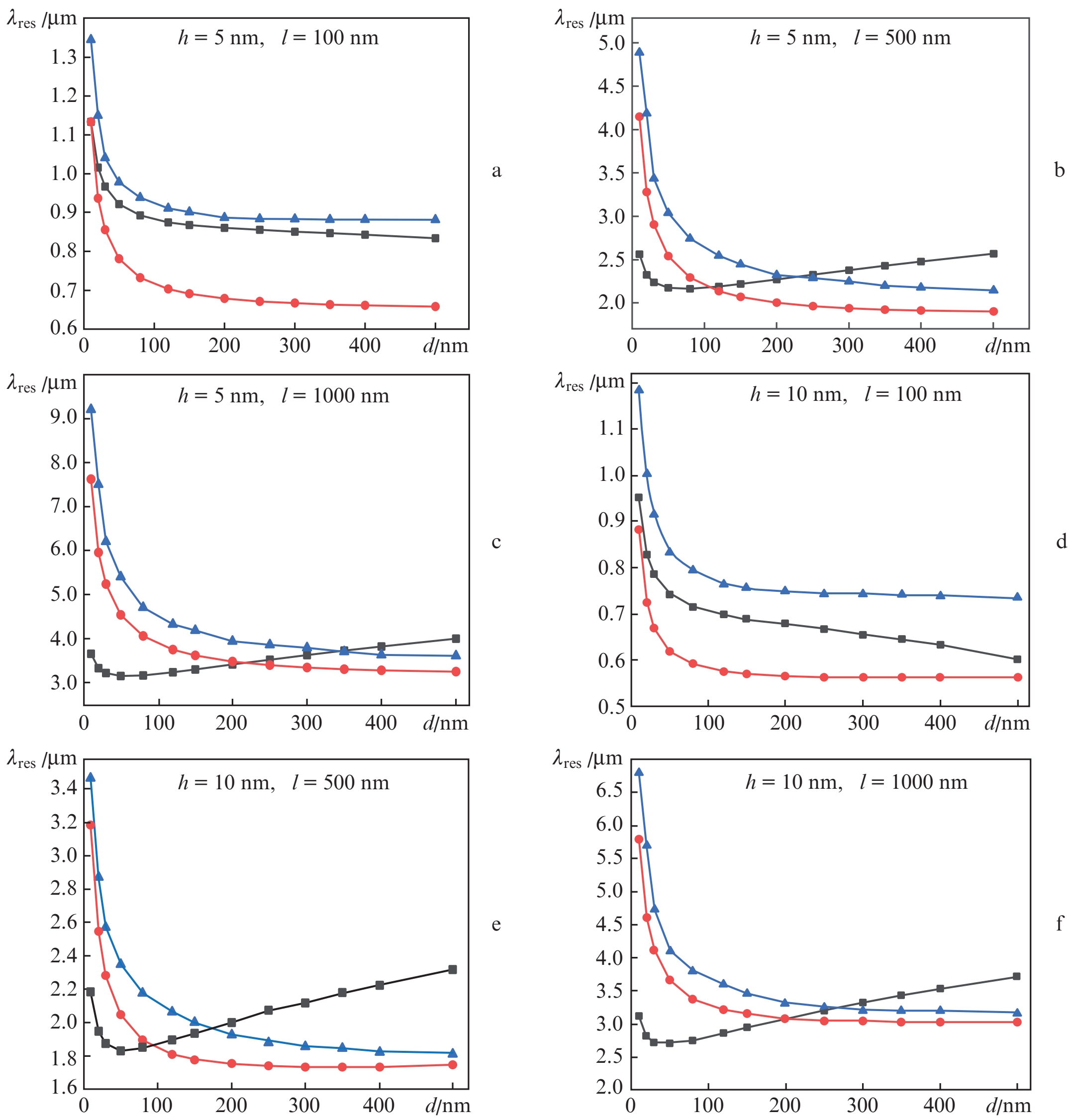

Figure 8. Dependences of the resonance wavelength on the width d of nanobars with l = (a, d) 100, (b, e) 500, (c, f) 1000 nm and h = (a–c) 5 and (d–f) 10 nm, calculated using the full-wave model in the Comsol environment (▲), the LCR model from Ref. [11] (■) and the refined LCR model of the present work (●).

antenna with the greatest length $l = 1000$ nm has the largest gradient in d.

4. Results and discussion

Let us analyse the applicability of the refined (as compared to Refs [10, 11]) LCR circuit model for quick estimation of the frequency response of a nanoantenna with a rectangular cross section. Figure 8 shows the dependences of the resonance wavelength on the nanobar widths with $l = 100, 500$ and 1000 nm and $h = 5, 10$ nm, obtained as a result of full-wave calculation in the Comsol medium, calculated using the model developed by the authors of Ref. [11] and the refined model proposed by the authors of this paper.

It can be seen that there are regions of nanoantenna parameters in which the model proposed by the authors of Ref. [11] provides very good agreement with the results of the full-wave calculation, but only for nanoantennas no longer than 100 nm. It should be noted that this coincidence was achieved in [11] by introducing a fitting factor of 2.5 to the electrical capacitance. In a wide range of parameters, the model [11] is not adequate, while the model, which takes into account the sinusoidal distribution of currents, maintains a relative error and correctly reflects the nature of the dependence in a wide range of nanoantenna parameters. Nevertheless, it is obvious that our model requires additional improvement and refinement to reduce the relative error of the calculation results. Inaccuracy may be due, e. g., to the influence of the uneven distribution of the field (current) over the width and thickness of the nanobar. In electrostatic problems, the charge density is high on the sharp edges of the conductor. Therefore, it can be expected that the current density increases near the edges of a wide nanobar. In the future, the authors intend to supplement the proposed methodology with allowance for the inhomogeneity of the field of currents over the cross section of the nanobar.

To summarise, the main results of this work include the following. Approximating formulas were obtained for calculating the resonance wavelength for a nanobar of rectangular cross section. Using the full-wave method, the dependences of the resonance wavelength on the width and thickness of the nanobar are obtained. Using approximating formulas, it is shown that the LCR model can be used to estimate the resonance frequency of nanoantennas with geometrical parameters varying over wide ranges. The ways to improve the LCR model are outlined.

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