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The Possibility of Managing the Width Of Resonance for Simple Single Nanoparticle

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Abstract. The paper demonstrates the possibility of a simple estimation of the resonance response expected frequency for a nanoantenna with the rectangular cross section when interacting with an external electromagnetic field. Additionally, the possibilities to construct a broadband resonance using scattering of nanoantennas with the rectangular cross section is analyzed. Analytical expressions for estimating of the resonance response are presented along with the full-wave modeling for rectangular nanoparticles with a thickness less than or equal to the thickness of the skin layer. Analytical expressions are obtained using the refined LCR-circuit model. The estimates are in good agreement with the results of the full wave modeling.

INTRODUCTION

There are many works focusing on the resonant response of metal and of dielectric nanoparticles to an external electromagnetic field. Specific interest for practical applications represents: the optical range, the near-IR range (telecommunication wavelengths) and the terahertz range. In addition to the resonant frequency (wavelength), an important characteristic is the quality factor of the resonance associated with its width. There is a class of problems for which a broadband resonant response is of special importance. The most obvious are the problems of broadband filtering in telecommunication technologies and the sensor problems, in which complex absorption spectra and the like are recorded against a background of wide plasmon resonance. To date, the research in the field of creating a broadband response has been intensive and several interesting works have been published recently aimed at constructing a basic scheme (geometry) for obtaining a broadband response for technological applications such as a polarization converter, a broadband absorber, controller of chromatic aberrations [1-4]. Nevertheless, the received broadband responses are strongly limited by the frequency range and are not homogeneous within each considered range.

Considering above it seems relevant to develop approaches for predicting and controlling the width of the plasmon resonance. In addition, one should consider the importance of the ease of applying nanoparticles to a solid substrate, in particular by the method of nanolithography in the manufacture of ordered meta-surfaces. The simplest

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in the production are nanoantennas which sections are close to rectangular or square, exactly such a geometry of individual nanoblocks was used in [1-4].

In our work, we investigate the possibilities and limitations of adjusting the width of the resonance for a single gold antenna in the optical and near-IR ranges.

It should also be noted that full-wave, especially three-dimensional, modeling of the resonance response of metasurfaces requires, at a minimum, large computational resources, so it would often be useful to be able to obtain plausible estimates for resonance characteristics, such as resonance frequency and resonance width (resonance quality factor) more easily. To build such a model, it makes sense to take as a basis the LCR-circuit model [5]. In this paper we analyze the possibilities of using such a model to obtain working analytical evaluation formulas.

It should also be noted that in the case of a rectangular antenna there are three independent parameters for tuning the resonance frequency and resonance width: length, width and depth. By fixing, for example, length and width, and changing the depth of the antenna, we can adjust the frequency of the resonance response, as shown in [6], where the dependence of the optical response of a nano-antenna of a cylindrical shape on the form factor, which is the ratio of the length of the cylinder to its diameter, was studied. In [6], an appreciable change in the response frequency was shown as a function of such a form factor, but the width of the resonance obtained was not included in the authors' priority consideration. For the geometry considered in this paper (Fig. 1.), two form factors can be introduced: the ratio of the length (l) to the thickness (h) and the ratio of the length (l) to the width (d). The appearance of another independent coordinate in the considered geometry gives an additional degree of freedom for the choice of the width of the resonance. In this paper we consider the normal fall of the external electromagnetic field on a nanoantenna made of gold up to 20nm thick which corresponds to the upper limit of the skin layer for the IR spectrum. In the following, considering a nano-antenna with a rectangular section, we shall call it as a nanobaulk for brevity. In the case of an antenna with a circular cross section, i.e. nanocylinder, this will be indicated in the text.

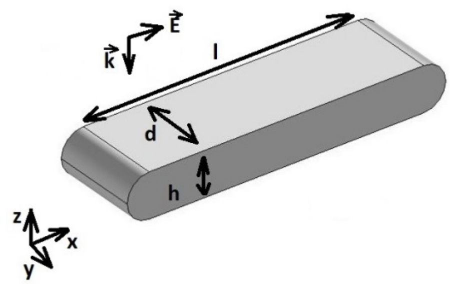


FIGURE 1. Gold nanobaulk

LCR – CIRCUIT MODEL FOR RESONANCE FEATURES ESTIMATIONS

In this paper we intend to compare the results of a full-wave calculation of the characteristics of light scattering by a gold nanobaulk and to estimate the scattering in a model where a nanobaulk is regarded as an electrical circuit of an oscillating circuit. Here it is worth noting that the optical frequency response of a nanoparticle or nanoantennas to external electromagnetic radiation is known to be due to factors such as the electrodynamic characteristics of the antenna, namely its capacitance and inductance. For the first time, the idea of considering a nanoobject as an oscillatory circuit was proposed in [7] to describe the resonance scattering of light by a gold nanosphere. In [8], such a light scattering object was a nanotube of the circular cross section, while the electric field strength was directed along the axis of the nanorod. In [8], a good agreement was obtained between the resonance wavelength of the light scattering in the LCR model of the circuit with the experimental results. In the same paper [8], a simple analytic formula was proposed for the resonant wavelength in the case of a nanorod replacement with a nanobaulk of rectangular cross section.

Considering that the calculation according to the formulas in [8] is in good agreement with other works for the nanorod, we assumed that to agree with the calculations for the nanobaulk, the formulas of [8] need to be refined somewhat, remaining within the LCR contour model. The main refinement is due to the modal composition of the resonances. In the simplest model [8], it is assumed that at each moment of time the current density is the same at all points in the volume of the nanorod and is directed along its axis. Nevertheless, as indicated by many authors, the current density at a given moment of time is proportional to the sinusoid, depending on the coordinate along the axis of the nanorod (or nanobaulk). At the nanorod ends the sinusoid goes to zero. Accordingly, for the lowest (dipole) mode, half of the wavelength of the sinusoid must fit within the length of the nanorod. This refinement of the LCR model has already been introduced by the authors of [9], in which the dipole mode is considered.

In [9], as in [8], L_0 is the nanoscale-specific contribution to the inductance of the circuit associated with the kinetic energy of electron drift motion. The L_0 value is the result of equating the kinetic energy to the inductance energy $L_0 I^2/2$, from which follows $L_0 = lm_e/Sne^2$, where l and S are the length and the cross-sectional area of the nano-sample, m_e is the electron mass, n is the conduction electron concentration in gold, and e is the electron charge modulus. The value of the expression ne^2/m_e can be obtained by relying on the well-known value of the plasma frequency for gold $\omega_p = \sqrt{ne^2/m_e\varepsilon_0}$. 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 $\delta = c/\omega_p = 21.9nm$ in accordance with [8] and [9] can be considered as the depth of penetration of the light field into gold. For comparison let's note that for optical frequencies the skin depth of the high-frequency electric currents is several times smaller than this value.

In addition to the contribution to the inductance of an equivalent oscillatory circuit specific to nanosamples L_0, there is also a traditional contribution to inductance L. In [9], as in [8], it is proposed to find this contribution in accordance with the definition of inductance

$$\frac{LI^2}{2} = \int\limits_{V=\infty} \frac{\mu_0 H^2}{2} dV \tag{2}$$

In [9] the capacity of the oscillatory circuit C is proposed to be found as

$$\frac{Q^2}{2C} = \int\limits_{V=\infty} \frac{\varepsilon_0 \varepsilon E^2}{2} dV \tag{3}$$

that is more correct compared to [8].

Completely agreeing with the formulas in [9] for calculating the capacitance and the traditional contribution to the inductance, we note that the integrals over an infinite volume can be replaced by integrals over the volume of the nanoobject, which greatly simplifies the calculations.

Indeed, for example, the energy of the electric field can be found as the energy of the conductor charges

$$\frac{Q^2}{2C} = \int\limits_{V=\infty} \frac{\varepsilon_0 \varepsilon E^2}{2} dV = \frac{1}{2} \int\limits_{V_0} \rho \varphi \, dV \tag{4}$$

where V_0 — nanoobject volume, $\varepsilon = n^2$ – the dielectric constant of the surrounding nanoobject medium with a refractive index n, ρ — bulk charge density, φ — potential,

$$\varphi(\vec{r}) = \frac{1}{4\pi\varepsilon_0\varepsilon} \int\limits_{V_0} \frac{\rho(\vec{r}\,')dV'}{|\vec{r} - \vec{r}\,'|} \tag{5}$$

As a result, taking into account the fact that the charge density is proportional to the cosine of the coordinate along the electric field $\vec{E}$ of the light wave, we obtain for the capacity of the mode with the number m

$$C = \frac{2\varepsilon_0 \varepsilon l}{\pi m^2 \int\limits_{V_0} \int\limits_{V_0'} \frac{\cos(m\pi x)\cos(m\pi x')}{|\vec{r} - \vec{r}\,'|} dV' dV} \tag{6}$$

where l — length of the nanobaulk along the field $\vec{E}$, V_0 and V_0' — the same volume of nanoobject, x and x' — the coordinate inside the nanoobject along the field $\vec{E}$, $\vec{r}$ and $\vec{r}\,'$ — radius vector of a point inside the nanoobject. The integrals are calculated in dimensionless variables where each coordinate is related to the length of the sample l.

Similarly, for inductance and magnetic field we obtain

$$\frac{LI^2}{2} = \int\limits_{V=\infty} \frac{\mu_0 H^2}{2} dV = \frac{1}{2} \int\limits_{V_0} jA\, dV \tag{7}$$

where j — the current density, A — vector potential,

$$\vec{A}(\vec{r}) = \frac{\mu_0}{4\pi} \int\limits_{V_0} \frac{\vec{j}(\vec{r}\,')dV'}{|\vec{r} - \vec{r}\,'|} \tag{8}$$

$$L = \frac{\mu_0 l}{2\pi} \int\limits_{V_0} \int\limits_{V_0'} \frac{\sin(m\pi x)\sin(m\pi x')}{|\vec{r} - \vec{r}\,'|} dV'dV \tag{9}$$

Here, same as for the capacitance, the integral is taken over the dimensionless variables related to the length of the sample l along the electric field $\vec{E}$ of the light wave.

Resonant frequency of the oscillatory circuit $\omega_r = 1/\sqrt{(L_0 + L)C}$ corresponds to the resonant wavelength

$$\lambda_r = 2\pi c/\omega_r = 2\pi c\sqrt{(L_0 + L)C} \tag{10}$$

where c — speed of light, C — capacitance.

Substituting expressions (1), (6), (9) into formula (10), we obtain the value of the resonance wavelength of the nanobaulk not only for the dipole mode (m = 1), as was done in [9], but for the mode with an arbitrary m.

According to our calculations, the dimensionless integrals in formulas (6) and (9) for the dipole mode (m = 1) are well approximated by the following formulas

$$\int_{C1} = \int\limits_{V_0} \int\limits_{V_0'} \frac{\cos(\pi x)\cos(\pi x')}{|\vec{r} - \vec{r}\,'|} dV'dV \approx \ln\left(1 + \frac{0.382}{\left(\frac{hd}{l^2}\right)^{0.585} \cdot \left(\frac{d}{h} + \frac{h}{d}\right)^{0.345}}\right) \tag{11}$$

$$\int_{L1} = \int\limits_{V_0} \int\limits_{V_0'} \frac{\sin(\pi x)\sin(\pi x')}{|\vec{r} - \vec{r}\,'|} dV'dV \approx \ln\left(1 + \frac{1.79}{\left(\frac{hd}{l^2}\right)^{0.515} \cdot \left(\frac{d}{h} + \frac{h}{d}\right)^{0.352}}\right) \tag{12}$$

that depend on m approximately as $\int_{Cm} = \int_{C1} \frac{a+1}{a+m}$ and $\int_{Lm} = \int_{L1} \frac{b+1}{b+m}$, where a and b — some parameters independent on m, dependent on nanobaulk form-factor; h — thickness of the nanobaulk in the direction of the wave vector of the incident light wave, d — width of nanobaulk, l — length of nanobaulk in the direction of the field $\vec{E}$ of the incident light.

The approximation of integrals (11) and (12) are valid within 5% for each of the pairs of values of the relative widths and thicknesses of the nanobaulk shown in Fig.2.

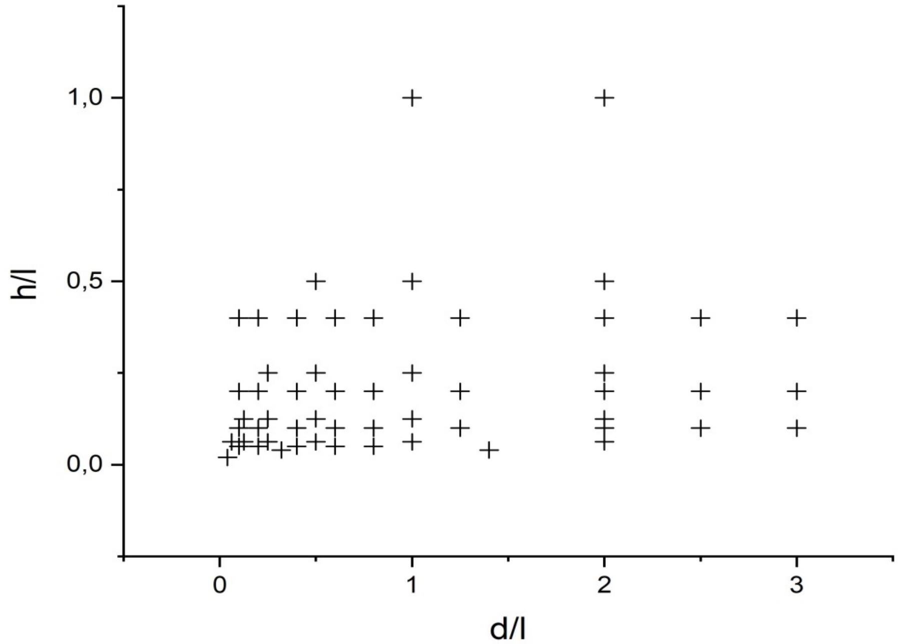


FIGURE 2. The range of nanobaulk shape factors in which the approximation (11) and (12) is checked by simple analytical formulas of integrals for inductance L and capacity C.

Formulas (1), (6), (9-12) allow to calculate the wavelengths of dipole resonance for a baulk in the entire range of practically interesting values in the LCR model of the circuit.

FULL-WAVE SIMULATION OF SINGLE NANOANTENNA WITH RECTANGULAR SECTION

As was mentioned above, the problem of the influence of one of the lengths, in particular of the thickness, on the position of the frequency of the resonant response of a cylindrical nanoantenna was studied in detail in [5]. The change in response frequency was shown depending on the diameter (thickness) of such a cylindrical nanobaulk. At the same time, the question of changing the width of the resonant response as a function of the diameter (thickness) of the nanocylinder was not considered. In this section, we present the results obtained by full-wave FTDT simulation for a nanobaulk with a rectangular cross section. Both the resonance frequency and the resonance width are analyzed as a function of the thickness (h) and the width of the nanobaulk (d) (Fig. 1).

FTDT Investigation of Nanobulk Resonance Response

Full-wave three-dimensional calculations for a nanoantenna with a rectangular cross section were made with the following parameters (Fig. 1). The length of the antenna was l = 500 nm, the thickness h was chosen based on the skin-layer dimensions. This choice of thickness is due to the fact that in the derivation of approximating analytical expressions by default, the existence of a uniform thickness distribution (along the z axis) was assumed. Electromagnetic responses of nanoantennas for h = 5, 10 and 20 nm were calculated. The width of the nanobaulk (d) varied from 20 to 900 nm. Below are the graphs (Fig.3) of the scattering cross section as a function of the length of the incident radiation. The graphs have a resonance character, the resonance corresponds to the first dipole mode. As the width of the nanobaulk increases, the resonant wavelength decreases, and the width of the resonance increases. On the left edge of the resonance, one can see a feature that is likely to be a resonance of the third mode. When the width of the nanobaulk changes, the resonances of the first and third modes move towards each other. Under normal incidence of light, the second mode is not excited.

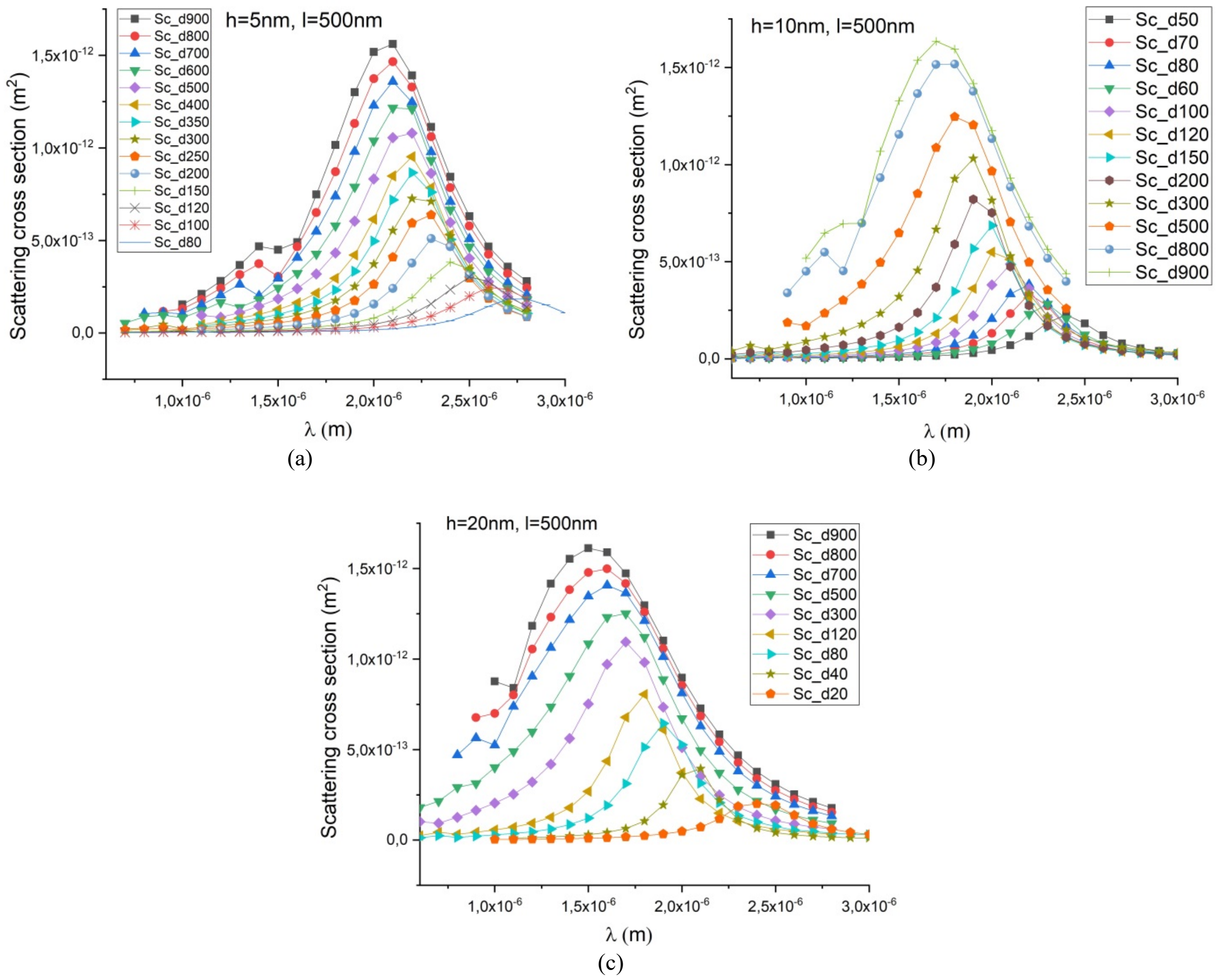
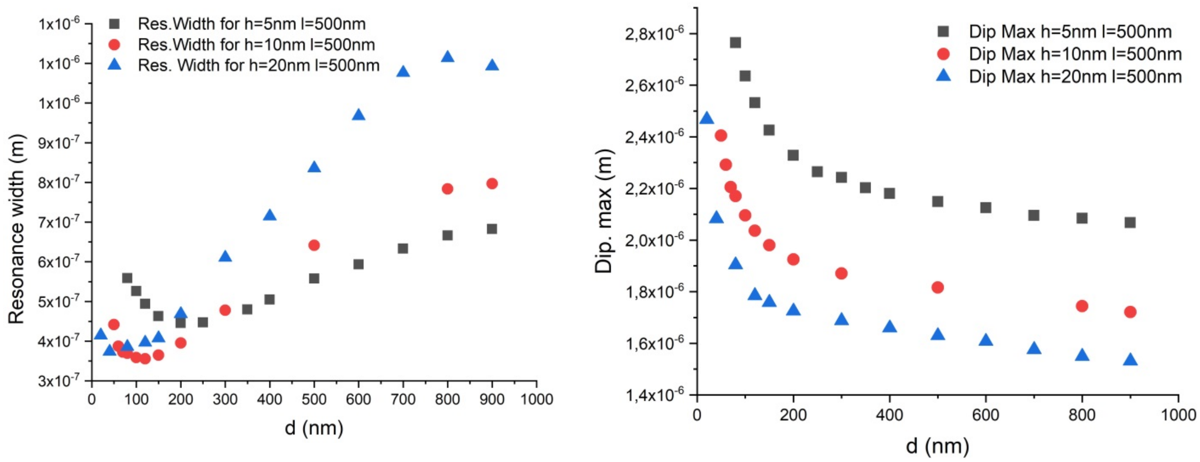


FIGURE 3. Scattering cross section depending on the incident radiation wavelength: (a) for h=5nm; (b) for h=10nm; (c) for h=20nm.

It is clearly seen from the graphs that in the chosen frequency range the first dipole mode has a resonant response. It is seen that with increasing nanobaulk width (d), the resonance frequency shifts to the region of shorter wavelengths and, consequently, to the high frequency region. In this case, starting from a certain size of nm, the resonant frequency remains practically unchanged. We also see the expected increase in the width of the resonance curve with increasing h and d.

Figure 4a shows plots of the resonance width versus the width of the nanobaulk d at h = 5, 10, 20 nm. It can be seen that the below dependences are essentially nonlinear. In addition, the following features can be observed: the dependence of the width of the resonance on the width of the beam has a minimum, for large values of d lying to the right of the minimum, the width of the resonance increases along with the increase of the beam thickness, and for small widths d of the nanobaulk (i.e. lying to the left of the minimum) the dependence is inverted.

Figure 4b shows the dependence of the value of the resonant wavelength on the width of the nanobaulk d from which it is seen that the resonance response has two characteristic regions: a nonlinear region of rapid change to about d approximately 300 nm and a linear region where the resonant wavelength varies very slowly with increasing d.



(a) (b)

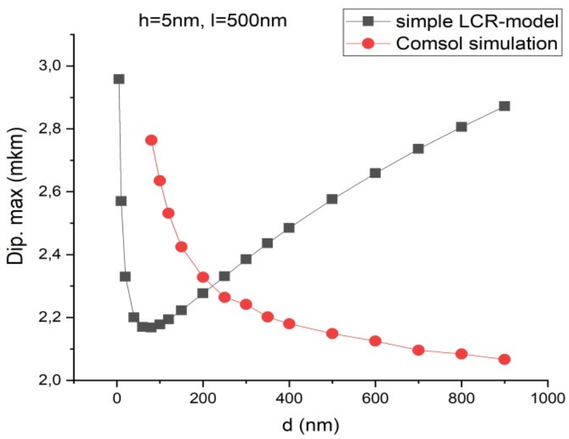
FIGURE 4. (a) the dependence of the width of the resonance on the width of the nanobaulk d at h = 5, 10, 20 nm; (b) the dependence of the value of the resonance wavelength on the width of the nanobaulk d.

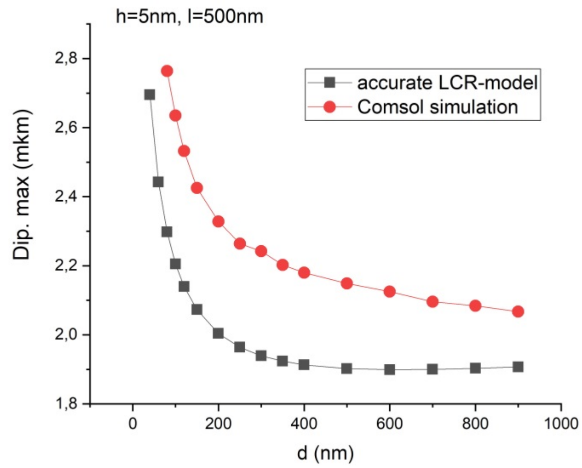
RESULTS AND DISCUSSION

In this section, we focus on comparing the results obtained with full wave modeling against the approximating formulas (11) and (12) we obtained within the framework of the LCR-circuit model. Here we analyze the adequacy of the analytical expressions obtained by considering resonant wavelengths without discussing the width of the resonance.

Figure 5 shows the dependence of the resonance wavelength on the width of the nanobaulk. The data are given for the nanobaulk length of 500 nm, thickness h = 5 nm. For thicknesses h = 10 and 20 nm the dependences are similar. With the full-wave calculation and the simplified formula for the LCR model, see [8]. As can be seen in Fig.5a, for a large nanobaulk width the discrepancy between full-wave calculation and the LCR-model is significant. Therefore, following the work [9], we refined the formulas of the LCR-model as described in the first part of this paper. The simpler expressions for integrals obtained by us and their analytical approximation allowed us to compare the full wave calculations and the refined LCR model. The results of this comparison are presented in Fig. 5b.

After refinement of the LCR-model, the nature of the obtained dependences for both full-wave calculation and for estimating by means of approximating formulas (11) and (12) completely coincide. Nevertheless, as is evident from Fig. 5b, the approximating model requires additional work and refinement. The difference can be caused, for example, by the influence of the uneven distribution of the field over the thickness of the nanobaulk. In the future, the authors propose to supplement the proposed technique by including consideration of the field and current inhomogeneities in the nanobaulk thickness.





(a) (b)

FIGURE 5. Dependence of the value of the resonant wavelength on the width of the nanobaulk d for full-wave calculation and the simplified formula of the LCR model
(a) comparison of full-wave calculations and calculations using the formula from [8] (b) comparison of full-wave calculations and refined LCR-model

Summarizing the above, the following results of this work may be articulated: obtained approximating formulas for the calculation of the resonant wavelength for a nanobaulk of a rectangular cross section, the dependency of the resonance wavelengths on the width and thickness of the nanobaulk were found both by the full-wave method and by using the approximating formulas, obtained dependence of the resonance loops width as a function of width and thickness of the nanobaulk. The authors have also demonstrated the possibility of using the LCR-model for estimating the resonance frequency and ways of refining the model.

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