

Electrodynamic approach for calculating the absorption spectra of plasmons in a rectangle with a two-dimensional electron gas excited by an incident electromagnetic wave

D. V. Fateev^{1,2}✉, K. V. Mashinsky²

¹Saratov State University, Russia

²Saratov Branch of Kotelnikov Institute of Radioengineering and Electronics of the Russian Academy of Sciences, Russia

E-mail: ✉fateevdv@yandex.ru, konstantin-m92@yandex.ru

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Abstract. The purpose of this research is to develop an electrodynamic method for calculating the plasmon spectrum in a three-dimensional structure with a two-dimensional electron gas excited by an incident electromagnetic wave. *Methods.* The developed method is based on solving integral equations formed with respect to induced currents in the conducting parts of a three-dimensional structure. *Results.* The convergence of the method and the calculation time were studied. The conditions for the convergence of calculations of higher plasmon resonances in a rectangular structure with a two-dimensional electron gas are determined. The normal incidence of an arbitrarily polarized electromagnetic wave on a rectangle with a two-dimensional gas is studied. The spectra of the absorption, extinction, forward and back scattering cross sections of the incident wave are calculated. *Conclusion.* It is found that in a rectangular structure containing a two-dimensional electron gas, the spectrum of plasmon resonances is modified in comparison with established by two-dimensional models of problem formulation, in which the structure is assumed to be infinite and homogeneous in one of the directions. It has been established that the incident wave most effectively excites fundamental plasmon modes. Plasmonic modes exhibit strong charge accumulation at the edges of the rectangle, which significantly affects the resonant excitation frequencies of plasmonic modes.

Keywords: integral equations method, plasmon, two-dimensional electron gas, terahertz.

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Introduction

Recently, there has been a wide interest in the creation of terahertz (THz) devices using two-dimensional plasmons for localization and amplification of electromagnetic fields and for

using the nonlinear properties of plasmons [1]. Traditionally, a two-dimensional electron gas is formed during the formation of a quantum well in the conduction band of semiconductor heterostructures. In micron and submicron field-effect transistors with a two-dimensional electron channel, it is possible to excite two-dimensional plasmons in the terahertz range [2]. Based on the properties of two-dimensional plasma waves, theoretical studies of THz plasmon effects are solved in a two-dimensional formulation of the problem, in which the direction perpendicular to the plasmon propagation is considered infinite and homogeneous [3, 4]. This formulation of the problem significantly simplifies the solution of dispersion problems and problems of plasmon excitation by an external electromagnetic wave. A simplified two-dimensional approach can be applied to plasmonic structures whose size in the direction transverse to the direction of plasmon propagation exceeds the wavelength of the terahertz plasmon by an order of magnitude or more. In principle, millimeter sizes are experimentally achievable in plasmonic structures created on the basis of semiconductor heterostructures. With a typical micron wavelength of the terahertz plasmon, the sizes of semiconductor heterostructures can reach several millimeters [5].

However, the sizes of the created plasmonic structures are often comparable with the sizes of short-wave plasmons, and the coupling with a long electromagnetic wave is carried out using additional antennas. In structures of such sizes, the influence of edge effects of induced fields on the response becomes significant, and sometimes dominant. Despite the impossibility of describing edge effects in a two-dimensional approach, new plasmonic physical effects were described with its help, such as plasmon-plasmon scattering [3, 6], an increase in the effective wavelength in plasmonic resonators, and radiative damping of plasmons. In this case, to solve the problem of excitation of plasmonic modes in a resonator of two-dimensional electron systems, it is necessary to take into account the electromagnetic delay.

The most studied three-dimensional structures are plasmonic structures with a symmetrical resonator shape of a two-dimensional system in the form of a circular disk (or ring) [7–12]. Much less work is devoted to the excitation of plasmons in a rectangular two-dimensional electron resonator [13–15]. A rectangular resonator has reduced symmetry compared to the disk (or ring) geometry, so the theoretical consideration becomes more complicated. Theoretical approaches used to study plasmonic excitations in rectangular plasmonic resonators employ commercial numerical solvers [14–16] or simplifying approximations [13]. Finite element methods face serious difficulties when applied to problems involving electromagnetic processes of very different scales. Such difficulties arise in the study of plasmonic structures in which the wavelength of the terahertz electromagnetic wave and the plasmon wavelength differ by two orders of magnitude.

In this paper, an algorithm for calculating and investigating the features of the spectra of plasmons excited by a normally incident electromagnetic wave in a rectangle with a two-dimensional electron gas is developed.

1. Method

The excitation of two-dimensional currents in a rectangle with a two-dimensional electron gas, onto whose plane an electromagnetic wave of arbitrary polarization is normally incident, is investigated. The length of the rectangle in the OX direction is denoted as w , the width in the OY direction is l , and the wave is incident on the rectangle in the OZ direction from medium 1 to medium 2. The OXY plane separates two half-spaces with different permittivities.

The developed method consists of the following stages. At the first stage, the electric and magnetic fields of the scattered waves are expanded into a double spatial Fourier integral in the OX and OY directions, and the dependence of the Fourier components on the z coordinate is

considered exponential. The E_x component of the electric field is shown as an example

$$E_x^{(1,2)}(x, y, z, t) = \exp(-i\omega t) \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} E_{x,q_x,q_y}^{(1,2)} \exp\left(ik_{z,q_x,q_y}^{(1,2)} z\right) \exp(iq_y y) \exp(iq_x x) dq_x dq_y, \quad (1)$$

where q_x and q_y are the components of the wave vectors of the Fourier harmonics in the plane of the rectangle, $k_{z,q_x,q_y}^{(1,2)}$ are the transverse components of the wave vectors of the Fourier harmonics in the media, and ω is the circular frequency of the wave. Maxwell's equations are solved in semi-infinite dielectric media surrounding a rectangle with a two-dimensional electron gas. To stitch the solutions in dielectric media, boundary conditions are used for the components of the electric and magnetic fields in the plane of the two-dimensional gas. Using Ohm's law, in which the two-dimensional electron gas is described by the Drude conductivity σ [3], integral equations are formed for the currents j_x and j_y in the two-dimensional gas:

$$j_x(x, y) = \sigma \int_{-l/2}^{l/2} \int_{-w/2}^{w/2} j_x(x', y') G_{q_x,q_y}^{xx}(x, x', y, y') dx' dy' + \sigma \int_{-l/2}^{l/2} \int_{-w/2}^{w/2} j_y(x', y') G_{q_x,q_y}^{xy}(x, x', y, y') dx' dy' + \sigma Z_{0x} E_{in,x}, \quad (2)$$

$$j_y(x, y) = \sigma \int_{-l/2}^{l/2} \int_{-w/2}^{w/2} j_x(x', y') G_{q_x,q_y}^{yx}(x, x', y, y') dx' dy' + \sigma \int_{-l/2}^{l/2} \int_{-w/2}^{w/2} j_y(x', y') G_{q_x,q_y}^{yy}(x, x', y, y') dx' dy' + \sigma Z_{0y} E_{in,y},$$

where $G_{q_x,q_y}^{mn}(x, x', y, y')$ are the kernels of the integral equations, $m, n = x, y$, Z_{0x} and Z_{0y} are the coefficients of coupling with the incident wave, $E_{in,x}$ and $E_{in,y}$ are the components of the amplitude of the electric field of the incident wave. The system of integral equations (2) is solved by the Galerkin method by expanding the unknown currents j_x and j_y into series in Legendre polynomials in the directions x and y . This allows us to transform the system of integral equations into an infinite system of algebraic equations with respect to the coefficients of the expansion of the currents. Taking into account the convergence, the expansion of the unknown currents into a double series in Legendre polynomials is truncated to a polynomial of order N

$$j_x(\chi'_x, \xi'_y) = \sum_{n,n_1=0}^N \beta_{n,n_1}^{(x)} P_{n_1}(\xi'_y) P_n(\chi'_x), \quad (3)$$

$$j_y(\chi'_x, \xi'_y) = \sum_{n,n_1=0}^N \beta_{n,n_1}^{(y)} P_{n_1}(\xi'_y) P_n(\chi'_x),$$

where $P_n(\chi'_x)$ are the Legendre polynomials, $\beta_{n,n_1}^{(x,y)}$ are the coefficients of the current expansion, (χ'_x, ξ'_y) are the spatial coordinates (x, y) reduced to the interval $[-1, 1]$. Each term on the

right-hand side of the equation with an unknown current (2) creates N^2 algebraic equations and, accordingly, N^2 unknown expansion coefficients. The matrix of the algebraic system consists of elements of the form

$$M_{n_1, r_1, n, r} = \sigma \frac{lw}{4\pi^2} i^{r_1+r} i^{n+n_1} (-1)^{n+n_1} W_{n_1, r_1, n, r} - \frac{\delta_{nr}}{2r+1} \frac{\delta_{n_1 r_1}}{2r_1+1}, \quad (4)$$

where

$$W_{n_1, r_1, n, r} = \int_{-\infty}^{+\infty} J_{n_1}^{(s)}\left(q_y \frac{a}{2}\right) J_r^{(s)}\left(q_y \frac{a}{2}\right) \int_{-\infty}^{+\infty} Z(q_x, q_y) J_n^{(s)}\left(q_x \frac{w}{2}\right) J_r^{(s)}\left(q_x \frac{w}{2}\right) dq_x dq_y, \quad (5)$$

where $Z(q_x, q_y)$ – the admittances of the system calculated from Maxwell's equations; $J_n^{(s)}\left(q_x \frac{w}{2}\right)$ – the spherical Bessel functions; (q_x, q_y) – the wave vectors in the Fourier representation; n, n_1 – the row indices of the matrix elements, r, r_1 – the column indices of the matrix elements (the indices n, n_1, r, r_1 take values from 0 to N). The total size of the square matrix M of the system of equations is $2N^2$.

The resulting system of algebraic equations for the unknown coefficients of the expansion of currents $\beta_{n, n_1}^{(x, y)}$ is solved by the Gaussian elimination method by reducing the system matrix to a triangular form. The calculated induced currents (3) allow us to determine the resonant electrodynamic properties of a rectangle with a two-dimensional electron gas.

To calculate the energy characteristics of the interaction of an electromagnetic wave and a rectangle of two-dimensional gas, it is necessary to represent the fields of scattered waves forward and backward as the sum of the fields reflected from a homogeneous interface between the media and the scattered field. For example, the component of the electric field in the 1st medium is written

$$E_x(x, y, z) = E_{x, R} \exp\left(ik_{z, 0, 0}^{(1)} z\right) + \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \tilde{E}_{x, q_x, q_y} \exp\left(ik_{z, q_x, q_y}^{(1)} z\right) \exp(iq_y y) dq_y \exp(iq_x x) dq_x, \quad (6)$$

where $E_{x, R}$ is the electric field of the wave reflected from a homogeneous interface between the media, and \tilde{E}_{x, q_x, q_y} is the amplitude of the Fourier components of the electric field of the wave scattered backwards. The average Umov-Poynting power flux will describe the outgoing waves scattered by the rectangle

$$P_{zR, T} = 2\pi^2 \iint_{\pm\omega\sqrt{\varepsilon_1\varepsilon_0\mu_0}} \left(\tilde{E}_{x, q_x, q_y} \tilde{H}_{y, q_x, q_y}^* - \tilde{E}_{y, q_x, q_y} \tilde{H}_{x, q_x, q_y}^* \right) dq_y dq_x. \quad (7)$$

We exclude the flows of waves reflected and transmitted through the interface between the media, and, using Maxwell's equations, we write the flows of scattered radiation by the rectangle backwards P_{zR} and forwards P_{zT} as

$$P_{zR, T} = 2\pi^2 \iint_{\pm\omega\sqrt{\varepsilon_1\varepsilon_0\mu_0}} \frac{\left| \tilde{E}_{x, q_x, q_y} \right|^2 (\varepsilon_0\varepsilon_{1,2}\mu_0\omega^2 - q_y^2) + \left| \tilde{E}_{y, q_x, q_y} \right|^2 (\varepsilon_0\varepsilon_{1,2}\mu_0\omega^2 - q_x^2)}{k_{z_{1,2}}^* \mu_0 \omega} dq_y dq_x + \\ + 2\pi^2 \iint_{\pm\omega\sqrt{\varepsilon_1\varepsilon_0\mu_0}} \frac{2\text{Re} \left(\tilde{E}_{x, q_x, q_y} \tilde{E}_{y, q_x, q_y}^* \right) q_y q_x}{k_{z_{1,2}}^* \mu_0 \omega} dq_y dq_x. \quad (8)$$

The absorbed electromagnetic power in a rectangle by oscillating currents can be calculated as

$$A = \operatorname{Re} \left(\frac{1}{\sigma(\omega)} \right) \int_{-w/2}^{w/2} \int_{-l/2}^{l/2} \left(|j_x(x, y)|^2 + |j_y(x, y)|^2 \right) dx dy, \quad (9)$$

and the power flux density of the incident wave is determined by the expression

$$P_{in} = \sqrt{\frac{\varepsilon_0 \varepsilon_1}{\mu_0}} \left(|E_{in,x}|^2 + |E_{in,y}|^2 \right). \quad (10)$$

The obtained energy characteristics allow us to calculate the absorption cross section $\alpha_{CS} = A/P_{in}$, the forward scattering cross section $\alpha_T = P_{zT}/P_{in}$, the backward scattering cross section $\alpha_R = P_{zR}/P_{in}$ and the extinction cross section $\alpha_{CS} = (A + |P_{zT}| + |P_{zR}|)/P_{in}$.

The convergence of the results of calculating the resonance characteristics is determined by comparing the calculated inductive currents obtained with a successive increase in the size of the system matrix. A separate necessary condition is the convergence of the calculation of the matrix elements, each of which is a double integration in the space of wave vectors in the directions of q_x and q_y . Numerical integration of each coefficient is performed taking into account the convergence and with the division of the integral in the wave space into two - inside the light cone at $q_x, q_y \leq \frac{\omega}{c} \sqrt{\varepsilon}$ and outside the light cone at $q_x, q_y > \frac{\omega}{c} \sqrt{\varepsilon}$, where ε – the largest permittivity of the surrounding media. Such a division is necessary because in subwave structures the emitted and decaying induced fields have spatial scales that differ by an order of magnitude or more.

The main difference between the developed method and the method used in two-dimensional problems is a significant slowdown in calculations due to the increase in the size of the matrix N^2 with an increase in the number of Legendre polynomials compared to the size of the matrix N in two-dimensional problems. Double integration in the momentum space, when calculating

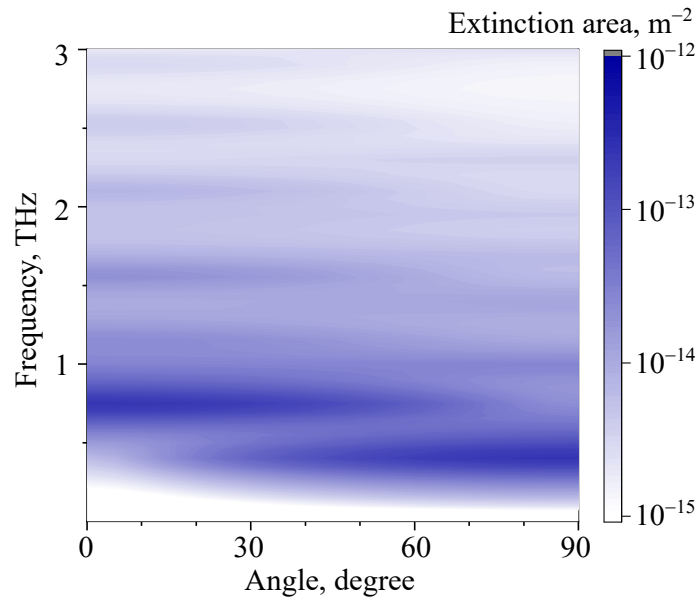


Fig 1. Dependence of the extinction cross-sectional area spectrum on the polarization angle of the electric field of a normally incident wave in a rectangle with dimensions $w = 1 \mu\text{m}$, $l = 2 \mu\text{m}$. A two-dimensional gas is described by Drude conductivity with the following parameters: electron momentum relaxation time 1 ps, electron density $2 \cdot 10^{11} \text{ cm}^{-2}$ and effective electron mass $0.067m_e$ (color online)

matrix elements also leads to a significant slowdown in calculations compared to one-dimensional integration when solving two-dimensional problems. In this regard, the calculation time for each matrix element of a three-dimensional problem also grows quadratically compared to a two-dimensional problem.

The calculated extinction area of a rectangle with a two-dimensional gas (Fig. 1) was obtained by performing the optical theorem with an error of 0.1%. The search for convergence of the solution showed the need to take into account 12 Legendre polynomials in the expansion of currents to study the first four plasmon resonances to achieve an error of 0.1%. A program in the Fortran programming language was created to perform the calculations. The calculations were performed on a personal computer with a 10-core processor. This made it possible to calculate the properties of the system at a given frequency in 15 seconds.

2. Results and discussion

Using the developed electrodynamic approach, the induced fields and currents in the structure were calculated, the spectra of the forward and backscattering cross-sections (Fig. 2), the absorption cross-section and the extinction cross-section (Fig. 2) were calculated for a rectangle of two-dimensional gas based on the AlGaAs heterostructure with dimensions $w = 1\mu\text{m}$, $l = 2\mu\text{m}$ (typical experimental structures are demonstrated in the works [5, 17]).

The calculated absorption cross section has a resonant character. This corresponds to the excitation of various plasmon modes in the structure. To identify excited plasmon modes, one can use a resonator model with ideally reflecting boundaries. In such a model, the wave vector of the plasmon mode will have discrete values $q = \sqrt{q_x^2 + q_y^2}$, where $q_x = \frac{\pi}{w}p$ – in the x direction and $q_y = \frac{\pi}{l}p_1$ – in the y direction, p and p_1 are integers. Therefore, each plasmon mode in the rectangle can be assigned two indices (p, p_1) .

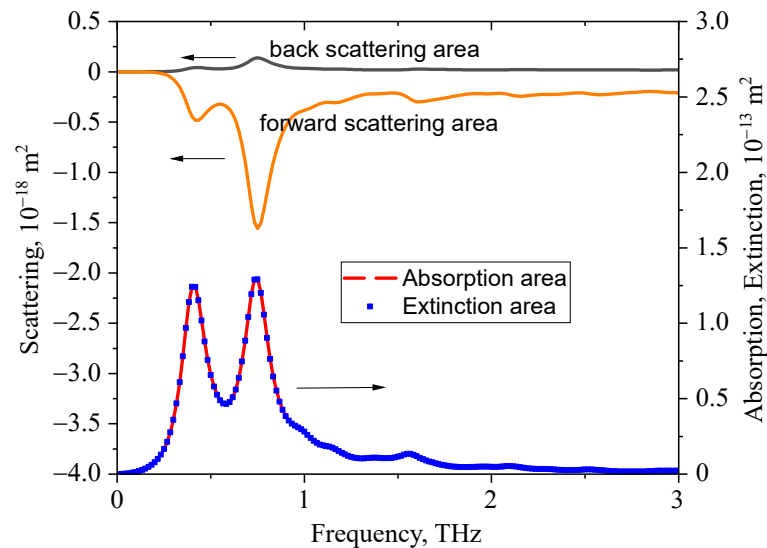


Fig 2. Spectra of the absorption cross section (red curve), extinction cross section (blue dots), backscattering cross section (black curve) and forward scattering cross section (green curve) for a rectangle with dimensions $w = 1\mu\text{m}$, $l = 2\mu\text{m}$. A two-dimensional gas is described by Drude conductivity with the following parameters: electron momentum relaxation time 1 ps, electron concentration $2 \cdot 10^{11}\text{ cm}^{-2}$ and effective electron mass 0.067. The electric field vector of the incident wave is directed at an angle of 45 degrees relative to the OX axis (color online)

To identify the modes, instantaneous distributions of the charge density oscillating in a rectangle with a two-dimensional gas are constructed. For this purpose, the linear charge density distribution for plasmon resonance in a rectangle with a two-dimensional gas is calculated using the continuity equation:

$$\rho = -\frac{i}{\omega} \left(\frac{\partial j_x}{\partial x} + \frac{\partial j_y}{\partial y} \right). \quad (11)$$

The charge density distributions at the plasmon resonance frequencies of 0.4009 THz, 0.7342 THz, 0.9675 THz and 1.551 THz (Fig. 3) are constructed, which allow us to draw conclusions about the structure of plasmon modes and identify them using the wavenumber discretization model. The plasmon at the frequency of 0.4009 THz corresponds to indices (0,1), at the frequency of 0.7342 THz – (1,0), at the frequency of 0.9675 THz – (2,1), and at the frequency of 1.551 THz – (1,2). The logarithmic plot of the extinction and absorption spectra shows that fundamental plasmon modes with indices (0,1) and (1,0) are most effectively excited

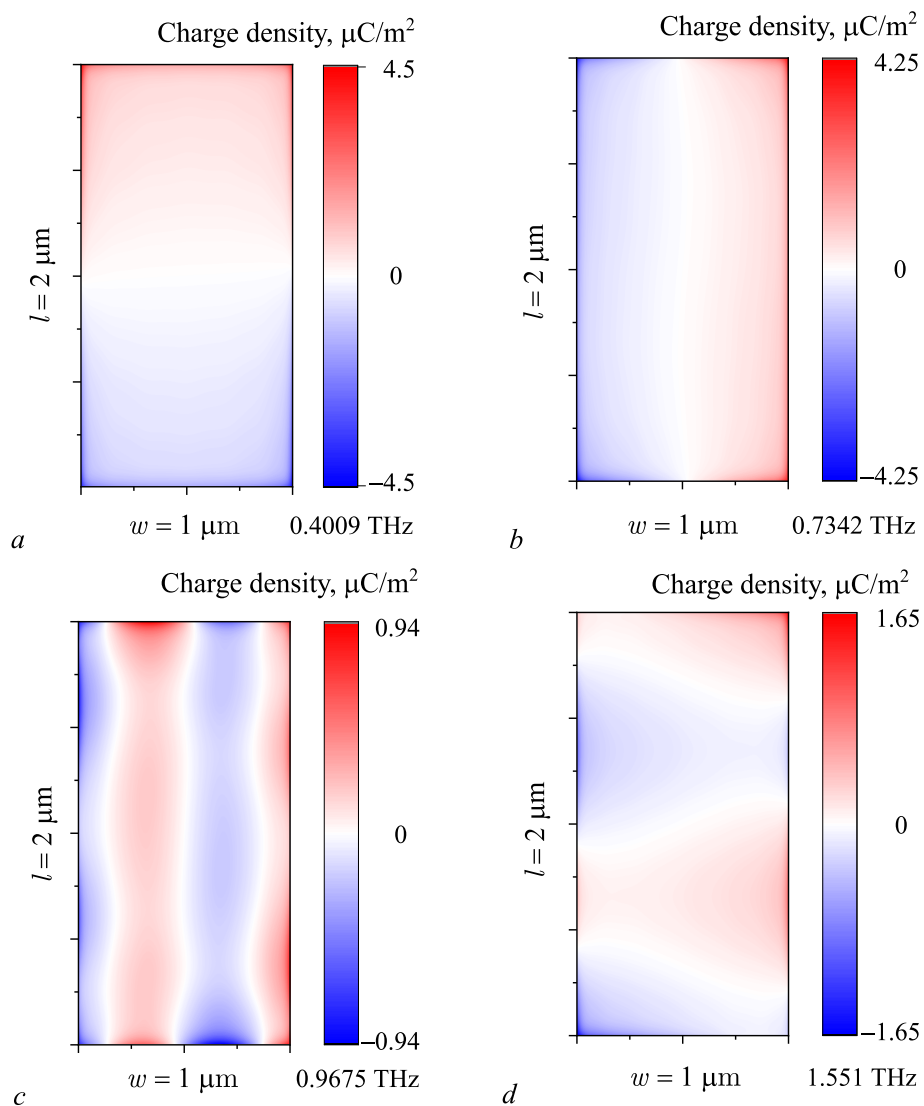


Fig 3. Charge density distribution in the plane of a rectangle with a two-dimensional electron gas in plasmon resonances corresponding to resonances in Fig. 1 at frequencies of 0.4009 THz (a), 0.7342 THz (b), 0.9675 THz (c) and 1.551 THz (d) (color online)

in the rectangle. However, for higher plasmon resonances the extinction cross section drops by an order of magnitude or more.

In Fig. 3 one can see a strong charge accumulation at the edges of the rectangle. This significantly affects the resonant frequencies of the plasmon modes compared to the frequencies predicted by simplified models. Such charge accumulation is associated with an increase in the electric field at the boundaries of the rectangle with a two-dimensional electron gas, leads to a significant field extension beyond the rectangle boundaries and reduces the resonant excitation frequencies of the plasmon modes.

The developed algorithm allows more accurate prediction of electromagnetic properties of a rectangle with a two-dimensional electron gas compared to commercial programs based on the finite element method, since it does not require placing the studied system in the solution domain. In this case, the modes of the solution domain are not mixed with the true solutions of the system under consideration. The proposed algorithm allows studying multilayer three-dimensional structures and solving problems with spatial dispersion in a two-dimensional electron gas that cannot be solved by finite element methods.

Conclusion

Thus, in this paper, an algorithm for calculating currents induced by an electromagnetic wave in a rectangle with a two-dimensional electron gas has been developed. The conditions for the convergence of the algorithm have been found and its performance has been compared with a similar algorithm for calculating plasmon properties in a two-dimensional problem statement. The absorption and extinction cross sections, as well as the spatial distributions of the charge density in plasmon resonances, have been calculated. It has been found that the incident wave excites fundamental plasmon modes with indices (0.1) and (1.0) most effectively. Plasmon modes demonstrate strong charge accumulation at the edges of the rectangle. This significantly affects the resonant excitation frequencies of plasmon modes.

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