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**RESONANCE SCATTERING OF ELECTROMAGNETIC WAVES BY FINITE
GRATINGS OF THIN METAL AND GRAPHENE STRIPS**

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SUMMARY

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GENERAL DESCRIPTION

This work is devoted to the development of efficient numerical method, having guaranteed convergence and controlled accuracy of computations, for the modeling of the resonance scattering of electromagnetic waves by finite gratings consisting of many thin material strips, and, on its basis, to the analysis of resonance effects in the scattering by finite gratings of dielectric strips independently of the range, noble-metal strips in the optical range, and graphene strips in the terahertz range.

Timeliness of research. In today's theoretical electromagnetics important place is occupied by the study of the scattering of waves by two-dimensional (2-D) models of various metal screens. In practice, such screens are frequently shaped as long thin strips and can be both flat and curved in the cross-sectional plane. In terms of modeling, this suggests assuming them infinitely long and, at least at microwaves, perfectly electrically conducting (PEC). Today the theory of the wave-scattering by infinitely thin PEC strips is well developed. Mathematically, the major advances are related to the integral-equation methods combined with analytical-regularization and Nystrom-type numerical algorithms. These algorithms allow solving the scattering problems with guaranteed convergence and controlled accuracy of computations.

Still general tendency of the development of today's electromagnetic-wave technologies is associated with much shorter-wavelength ranges including terahertz, infrared, and visible light. In these ranges and even in the optical range the dimensions of the elements of various devices are now comparable to the wavelength, which makes the ray-tracing methods unsuitable for modeling. The shape of these elements is often strip-like. However, the PEC model is not valid even for the scatterers made of noble-metals such as silver or gold in the mentioned wavelength ranges. Furthermore, in the visible range the dielectric permittivities of noble metals take complex values with negative real parts.

Today, nanotechnologies and nanomaterials is a constantly expanding area of science and industry that rapidly generates new directions such as nano-optics, nanophotonics, and nanoelectronics. Resonance effects in the scattering and absorption of electromagnetic waves by nanoscale metal objects are mainly associated with the excitation of localized surface plasmon resonances and have a wide range of practical applications. For example, in the development of biosensors plasmon effects allow to significantly enhance the possibility of detection, identification, and diagnosis of the biological substances due to the increasing of scattering or fluorescence intensity.

The individual metal and dielectric nanostrips are very attractive as components of optical nanoantennas and sensors due to their important features like planar geometry, conformability, simplicity, low cost of production, and availability of novel manufacturing technologies such as etching and molecular-beam epitaxy. Further, periodic arrays or gratings made of noble-metal nanosize elements are attracting even greater attention of research community. This is caused by the effects of extraordinarily

large reflection, transmission, emission, and near-field enhancement that have been found in the scattering of light by periodic nanosize scatterers. More broadly, these specific resonances display a variety of Fano shapes near to Rayleigh anomalies of associated infinite gratings. Here, truly large periodic arrays remain much less studied scatterers than individual strips or small collections of them, because of a lack of adequate tools of reliable and efficient numerical analysis.

The computational methods used for the modeling of the scattering and absorption characteristics of thin material strips and, in particular, optical nanostrips include volume and boundary IEs, where the integration domain is the area of the strip cross-section and its closed contour, respectively. Here, boundary IEs are considered more efficient as they imply the discretization of the boundary instead of the area; still typical number of unknowns is in hundreds and thousands, respectively. More essentially, boundary IEs can be cast, unlike volume IEs, to the forms having non-singular and integrable kernels and thus can be discretized more reliably. Still many forms of the boundary IEs possess spurious eigenvalues; this spoils the performance of the boundary IEs for the strips wider than half-wavelength of the incident light that corresponds to the first spurious eigenvalue for a strip of sub-wavelength thickness. To avoid this, one should use so-called Muller's boundary IE; still the shape of the contour and its non-smoothness greatly affects the rate of convergence of corresponding algorithms. All mentioned becomes still more important for grating consisting even of 10 or 20 strips.

Thus, the task of the building of new models to study the electromagnetic wave scattering by finite gratings consisting of large number of thin material strips (dielectric, noble-metal in the optical range, and graphene in the terahertz range) and development of the efficient numerical methods with guaranteed convergence and controlled accuracy of computations in a relatively short time is still timely and important.

Relation to R&D programs and projects. The research related to the thesis has been done in the framework of the following projects:

1. R&D project of the National Academy of Sciences of Ukraine (NASU) "Development and application of new methods of optics and quasioptics for investigation of the THz radiation interaction regularities and features with physical and biological objects" (code Oreol, #01.11U010479, 2012-2014).
2. State Target Program "Nanotechnologies and nanomaterials," project #1.1.3.45, "Fundamental mathematical and numerical study of optical electromagnetic fields of stand-alone and coupled microcavity lasers with nanosize active layers, wires and strips" (code Svitlo, #01.10U004737, 2010-2014).
3. Research and Networking Programme «NewFocus: New frontiers in millimeter and sub-millimeter wave integrated dielectric focusing systems» of the European Science Foundation, project "Resonance effects in the optical and terahertz antennas shaped as finite comb-like gratings of noble-metal nanostrips" (2012) together with the École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland.

4. Exchange program between NASU and the Academy of Sciences of Czech Republic (ASCR) via joint project «Electromagnetic and numerical modelling of active and nonlinear microcavities for semiconductor lasers and all-optical switches» (2010) with the Institute of Photonics and Electronics of ASCR, Prague, Czech Republic.
5. Research and Networking Programme «Plasmon-Bionanosense: New approaches to biochemical sensing with plasmonic nanobiophotonics» of the European Science Foundation, project «Modeling of optical nanoantennas shaped as comb-like metal strip gratings: interplay of surface plasmon resonances and periodicity-induced grating resonances» (2013) together with the Institute of Photonics and Electronics of ASCR, Prague, Czech Republic.

It has been also partially supported by the following international fellowships and scholarships:

- “Scattering from material and impedance strips analyzed using a Nystrom-type algorithm,” IEEE Antenna and Propagation Society (2010);
- “Optical nanoantennas made of thin noble-metal strips: integral equation modeling,” International Visegrad Fund, EU jointly with the Institute of Photonics and Electronics of ASCR, Prague, Czech Republic (2012-2013).

Aims and problems. The aims of the thesis research are the investigation of the regularities and specific features of the H- and E-polarized electromagnetic plane wave scattering by finite gratings consisting of large number of thin material strips – dielectric, noble-metal in the optical range, and graphene in the THz range. First of all, this needs the building of efficient and accurate 2-D model of the H- and E-polarized electromagnetic wave scattering by a thin stand-alone material strip. To this end, we propose using the two-side generalized boundary conditions (GBC) derived earlier to study thin dielectric scatterers. Based on this model, we develop innovative numerical algorithms for solving the corresponding singular and hyper-singular integral equations (IE) and systematically compute the far-field and near-field scattering and absorption characteristics. Proposed numerical algorithm is based on the Nystrom-type method and special quadrature formulas of interpolation type, adapted to the edge behavior. To achieve these goals, the following separate tasks have been considered:

- building of 2-D model of the H- and E-polarized electromagnetic wave scattering by a thin stand-alone material strip using the two-side GBC that allows to reduce the scattering problem to a set of two 1-D singular and hyper-singular IEs;
- generalization of the mentioned above 2-D model of the H- and E -polarized electromagnetic plane wave scattering to cover finite gratings of thin material strips (dielectric, noble-metal in optical range, and graphene in the THz range);
- development of efficient numerical algorithms for computations of the scattering and absorption cross-sections and field patterns in the far and near zones;
- accurate numerical analysis of the electromagnetic characteristics of various finite strip gratings in the context of the refractive-index sensing.

The object of research is the phenomena of the scattering and absorption of the H- and E-polarized electromagnetic plane waves by the finite gratings consisting of

- dielectric strips independently of the wavelength range;
- noble-metal nanostrips (silver or gold) in the optical range;
- graphene micro-size strips in the THz range.

The subject of research is the resonance effects in the scattering and absorption of the H- and E-polarized electromagnetic waves by finite strip gratings.

Methods of research. We have used several contemporary mathematical and numerical methods of the theory of electromagnetic-wave boundary value problems. For the modeling of the H- and E-polarized electromagnetic wave scattering by thin dielectric or noble-metal strips we have used the two-side GBC and known behavior of the electric and magnetic current components at the strip edges; for graphene strips we have used the resistive-sheet boundary conditions with complex-valued resistivity. The formulated 2-D problems have been reduced to sets of the 1-D singular and hyper-singular IEs for the unknown densities of electric and magnetic currents induced on the strips. To solve the obtained IEs we have used the Nystrom-type method and quadrature formulas of interpolation type that guarantee convergence and controlled accuracy of computations.

Scientific novelty of obtained results is determined by the novelty of the formulated problems, the developed methods and numerical algorithms, and the revealed physical effects. More specifically, we imply the following:

- a mathematically grounded 2-D model of the H- and E-polarized electromagnetic plane wave scattering by thin material (dielectric, noble-metal in the optical range, and graphene in the THz range) strips and their finite gratings has been built, for the first time, on the basis of the GBC and reduced to the equivalent sets of the 1-D singular and hyper-singular IEs; a thorough verification has been performed;
- a novel numerical algorithm for solving the corresponding singular and hyper-singular IEs using Nystrom-type method with the aid of the quadrature formulas of interpolation type that guarantees convergence and controlled accuracy of computations has been developed;
- physical regularities of the influence of the geometrical and material parameters (strip width and thickness, grating period, and strips' number) on the scattering and absorption characteristics have been revealed;
- the nature and features of the surface plasmon resonances of the primary and higher orders for nanosize noble-metal strip gratings in the optical range and microsize graphene strip gratings in the THz range have been studied;
- the grating resonances, induced by the periodicity, in the scattering and absorption of the H-polarized plane waves by finite gratings consisting of thin noble-metal strips, have been found and their properties in dependence on the geometrical and material parameters have been investigated for the first time;

- mutual influence of the resonances on the localized surface plasmons and on the grating modes has been analyzed;
- refractive-index sensitivities of the optical resonances of various types on the finite comb-like silver-strip nanogratings have been computed for the first time.

Practical importance of obtained results. The proposed approach and the developed numerical algorithms can be used for the accurate and time-efficient computation, using the moderate computer hardware, of the H- and E-polarized plane wave scattering and absorption by finite gratings consisting of tens or hundreds of thin material strips (dielectric, noble-metal in the optical range or graphene in the THz range).

Obtained numerical results cover the characteristics of the resonance scattering and absorption of the visible light and terahertz waves by such gratings and have a wide range of applications. Strips and their finite gratings are very attractive as basic components in the design of many microwave, terahertz, and optical devices (nanoantennas, biosensors, solar cell absorbers, etc.). Plasmon resonances on the individual noble-metal and graphene strips can significantly enhance the detection, identification and diagnostic possibilities of the biological objects by increasing the intensity of the scattering or fluorescence. Finite strip gratings and associated high-Q grating resonances find their application in optical biosensors due to the enhanced reflection, emission, and near-field enhancement effects. The analysis of mutual influence of the plasmons and the grating resonances deepen the understanding of the resonance properties of finite strip gratings. This makes them promising for the development of new optical components with significantly improved characteristics.

High efficiency of the developed algorithms in the computation of the main scattering and absorption characteristics allows using them as a core of software for numerical optimization of optical nanoantennas, key elements of which are thin strips,.

Personal contribution of the candidate. All main results presented in the thesis have been obtained by the author. Her contribution, in the co-authored papers [1-16], is in the derivation of the basic equations, development of numerical algorithms, systematic computing of the scattering and absorption characteristics, far and near-field patterns and also interpretation of the obtained numerical results. In the review papers [2] and [8], it is the derivation of basic equations and computation of the numerical results for the electromagnetic plane wave scattering by a finite silver strip grating in the optical range and by a stand-alone graphene strip in the THz range, respectively.

Dissemination of results. The thesis results have been reported and discussed at the following scientific seminars: IRE NASU (Prof. P.M. Melezhik), Institute of Photonics and Electronics of ASCR, Prague, Czech Republic (Prof. J. Ctyroky), Ecole Normale Supérieure de Cachan, Cachan, France (Dr. M. Lebental), Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland (Prof. J. Mosig), Tokyo University of Technology,

Tokyo, Japan (Prof. M. Ando), Nihon University, Tokyo (Prof. T. Yamasaki). They were also presented at the following international conferences and symposia:

- International Symposium on Physics and Engineering of Microwaves, Millimeter and Sub millimeter Waves, Kharkiv (2010)
- International Conference on Transparent Optical Networks, Munich (2010), Stockholm (2011), Cartagena (2013)
- International Conference on Mathematical Methods in Electromagnetic Theory, Kyiv (2010), Kharkiv (2012)
- International Conference on Laser and Fiber-Optic Numerical Modelling, Sebastopol (2010), Kharkiv (2012), Sudak (2013)
- Asia-Pacific Radio Science Conference, Toyama (2010)
- International Workshop on Theoretical and Computational Nanophotonics, Bad Honnef (2011)
- European Conf. on Antennas and Propagation, Prague (2012), The Hague (2014)
- International Conference on Near-Field Optics, San Sebastian (2012)
- International Symposium on Antennas and Propagation, Nagoya (2012)
- International Conf. Electronics and Nanotechnology, Kyiv (2013, 2014)
- URSI Commission B Symposium on Electromagnetic Theory, Hiroshima (2013)

Publications. The results of research have been published in 24 papers including 8 papers in technical journals [1-8] and 16 papers in the proceedings and digests of the international conferences, the main of which are [9-16].

Structure and length of thesis. The thesis includes an introduction, 5 chapters, conclusions, and a list of literature sources used. The total thesis size amounts 198 pages, from which 14 pages are for the list of references (184 entries).

THESIS CONTENTS

In introduction, the timeliness of the considered topic is grounded, the aim and the tasks of the investigation are formulated, and the general characteristics of thesis are presented.

Chapter 1 is an overview of the literature published around the topic of dissertation. It provides also general information about various applications of the models of zero-thickness PEC, imperfect-metal, dielectric, and graphene strips and their periodically structured configurations in physics and engineering of microwaves, millimeter, sub-millimeter, and terahertz waves and also waves of the visible range.

First of all, an overview of theoretical approaches, techniques and methods used to solve the electromagnetic-wave scattering by infinite gratings of PEC and resistive strips is presented. Major attention is paid to the mathematically grounded methods of analytical regularization and Nystrom-type interpolation, which guarantee convergence

and controlled accuracy of computations. Significant contributions to this area belong to Marchenko, Sologub, Sirenko and Gandel, Nazarchuk, Tsalamenhas, respectively.

However, the general tendency of the development of electromagnetic-wave physics and technology is associated with the mastering of shorter-wavelength ranges including terahertz and infrared where the model of PEC is no longer suitable. Indeed it does not allow taking into account the ohmic losses which always occur in realistic imperfect objects. Next an overview of the volume and the boundary IEs methods used in the modeling of the scattering by thick stand-alone material strips and, in particular, optical nanostrips is provided. The actuality of the development of new models and methods to study the scattering of electromagnetic waves by finite gratings consisting of a large number of thin material strips (dielectric, noble-metal in the optical range, and graphene in the THz range) and corresponding numerical algorithms with guaranteed convergence is justified. Finally, a detailed overview of the two-side GBC derived in the 1960's-1990's from the rigorous analysis of the problem of electromagnetic plane wave scattering by infinite homogeneous material slab of thickness h under the condition $k_0 h \ll 1$, is presented. This GBC has the following generic form:

$$\left[E_{tg}^+ + E_{tg}^- \right] = 2Z_0 R \cdot \vec{n} \times \left[H_{tg}^+ - H_{tg}^- \right], \quad \left[H_{tg}^+ + H_{tg}^- \right] = -2Z_0^{-1} Q \cdot \vec{n} \times \left[E_{tg}^+ - E_{tg}^- \right], \quad (1)$$

where \vec{n} is the unit vector normal to the strip top side, the indices \pm correspond to the limit values of the field at the top and bottom sides of the strip, k_0 is the free-space wavenumber, and Z_0 is the impedance of the free space. The coefficients R and Q are called the electric and magnetic resistivities, which have several forms depending on the slab material. If the electric contrast is high, $|\varepsilon_r \mu_r| \gg 1$, then

$$R = 0.5i\sqrt{\mu_r / \varepsilon_r} \operatorname{ctg}(k_0 h \sqrt{\varepsilon_r \mu_r} / 2), \quad Q = 0.5i\sqrt{\varepsilon_r / \mu_r} \operatorname{ctg}(k_0 h \sqrt{\varepsilon_r \mu_r} / 2). \quad (2)$$

If, alternatively, the contrast is low, $k_0 h |\varepsilon_r - 1| \ll 1$, then

$$R = i[k_0 h (\varepsilon_r - 1)]^{-1}, \quad Q = i\varepsilon_r [k_0 h (\varepsilon_r - 1)]^{-1}. \quad (3)$$

The GBC (1) is approximate, however it is clearly a large step ahead from the PEC condition, to which it turns if $R = 0$ and $Q = \infty$. A modified (compensated) version of GBC (1) that keeps validity for $\varepsilon_r \rightarrow 1$ by taking into account the compensation for the reduction of the slab area to the line of zero thickness has been proposed recently as

$$\tilde{R} = \frac{\mathcal{G} - R - \mathcal{G}^2 R}{4\mathcal{G}R - \mathcal{G}^2 - 1}, \quad \tilde{Q} = \frac{\mathcal{G} - Q - \mathcal{G}^2 Q}{4\mathcal{G}Q - \mathcal{G}^2 - 1}, \quad (4)$$

where $\mathcal{G} = i \cot(k_0 h / 4)$, and R and Q are taken from (2).

Further, the applicability limits of the GBC have been demonstrated with the aid of the relative error calculation of the reflection coefficient for the H-polarized plane wave scattered by a thin infinite dielectric slab. Here the values obtained using the GBC-based models were compared to their precise values. It has been shown that the relative error of the compensated GBC does not exceed 1.5% for $k_0 h \leq 0.1$.

The second chapter is devoted to building an efficient numerical algorithm for the H- and E-polarized electromagnetic plane wave scattering and absorption by a stand-alone dielectric strip of the width d and the thickness h (Fig. 1). Assuming the strip to be thinner than the wavelength $h \ll \lambda$ ($k_0 h \ll 1$) and by neglecting the internal field and considering only the external field limit values, we shrink strip's cross-section $S = \{(x, y) : 0 \leq x \leq d, -h/2 \leq y \leq h/2\}$ to the median line $L = \{(x, y) : 0 \leq x \leq d, y = 0\}$ where the two-side GBC (1) are imposed.

Here, for the building of the 2-D scattering model, we use the Maxwell equations, the above mentioned GBC, the condition of local finiteness of power, and the radiation condition at infinity. Together they guarantee the uniqueness of the solution of the formulated scattering problem. The known behavior of the electric and magnetic current components approaching the edges of the resistive strip is also exploited.

The scattered field outside of the strip is sought as a linear combination of the single-layer and double-layer potentials,

$$U_{sc}(\vec{r}_0) = k_0 \int_L v(\vec{r}) G(\vec{r}, \vec{r}_0) d\vec{r} + \int_L w(\vec{r}) \frac{\partial G(\vec{r}, \vec{r}_0)}{\partial \vec{n}(\vec{r})} d\vec{r}, \quad (5)$$

where $G(\vec{r}, \vec{r}') = (i/4)H_0^{(1)}(k|\vec{r} - \vec{r}'|)$ is the 2-D Green function. Note that the unknown functions $v(\vec{r}) = [\partial H_z^+(\vec{r}) / \partial \vec{n}(\vec{r}) - \partial H_z^-(\vec{r}) / \partial \vec{n}(\vec{r})]$ and $w(\vec{r}) = [H_z^+(\vec{r}) - H_z^-(\vec{r})]$ are the magnetic and electric surface currents, respectively, induced on the strip.

Using (5) in GBC (1), the boundary problem is reduced to two independent singular and hyper-singular IEs of the second kind for the unknown functions $v(\vec{r})$ and $w(\vec{r})$, respectively. Finally, after introducing the strip median-line regular parameterization as $x = x(t)$, $y = y(t) \equiv 0$ for $t \in [-1, 1]$, taking into account the behavior of the current components while approaching the strip edges, and using new unknown smooth function $\tilde{w}(t)$, where $w(t) = \tilde{w}(t)\sqrt{1-t^2}$ for all $t \in [-1, 1]$, we obtain the following IEs:

$$\frac{4}{\kappa} Q v(t_0) + \frac{2i}{\pi} \int_{-1}^1 v(t) \ln |t - t_0| dt + \int_{-1}^1 v(t) M_v(\kappa, t, t_0) dt = f_v(\kappa, t_0), \quad (6)$$

$$4R\tilde{w}(t_0)\sqrt{1-t_0^2} + \frac{i\kappa}{\pi} \int_{-1}^1 \tilde{w}(t)\sqrt{1-t^2} \ln |t - t_0| dt + \frac{2i}{\pi\kappa} \int_{-1}^1 \frac{\tilde{w}(t)}{(t - t_0)^2} \sqrt{1-t^2} dt + \int_{-1}^1 \tilde{w}(t)\sqrt{1-t^2} M_w(\kappa, t, t_0) dt = f_w(\kappa, t_0), \quad \text{for all } -1 < t_0 < 1, \quad (7)$$

where $M_v(\kappa, t, t_0)$, $M_w(\kappa, t, t_0)$, $f_v(\kappa, t_0)$ and $f_w(\kappa, t_0)$ are known smooth functions for all $-1 \leq t \leq 1$, and $\kappa = k_0 d / 2$ is the normalized frequency. Note that integral operator of the hyper-singular IE (7) should be understood in the sense of Hadamard's finite part.

The solutions of the obtained IEs (6) and (7) are sought in the form of interpolation polynomials of the degrees of $n_v - 1$ and $n_w - 1$, respectively. We isolate the singularities and discretize the resulting sets of IEs using the Nystrom-type method with two different quadrature rules of interpolation type, adapted to the edge behavior of the unknowns:

- Gauss-Legendre quadrature formulas of the n_v -th order for IE with logarithmic singularity (6), with the nodes in the nulls of the Legendre polynomials, $\{\tau_k\}_{k=1}^{n_v} : P_{n_v}(\tau_k) = 0, k = 1, 2, \dots, n_v$;
- weighted quadrature formulas of the n_w -th order of interpolation type (with weight $\sqrt{1-t^2}$) for hyper-singular IE (7) with the nodes in the nulls of the Chebyshev polynomials of the second kind, $\{t_j\}_{j=1}^{n_w} : t_j = \cos(j\pi / (n_w + 1)), j = 1, 2, \dots, n_w$.

As the collocation nodes, we take the corresponding discretization nodes.

Finally, by applying the above mentioned quadrature formulas, the boundary problem is equivalently reduced to two independent sets of matrix equations of the orders n_v and n_w for the values $\{v(\tau_k)\}_{k=1}^{n_v}$ and $\{\tilde{w}(t_k)\}_{k=1}^{n_w}$, respectively. These matrix equations represent discrete models of IEs (6) and (7). On solving them numerically the approximate solutions of IEs in the form of interpolations polynomials for the unknown surface currents are obtained. The chosen quadrature formulas ensure rapid convergence of numerical solutions to the accurate ones if $n_v, n_w \rightarrow \infty$. Conservative estimation gives the rates of convergence as $O(1/n_{v,w})$, although the actual rate is always greater.

In terms of the quadrature formulas of interpolation type the approximate expressions for the magnetic and electric fields at an arbitrary point of the space and far-field patterns with main scattering and absorption characteristics are obtained.

Besides, we have investigated the scattering and absorption characteristics of the H- and E-polarized plane wave scattering by dielectric strips with losses and relatively large real parts of dielectric permittivity. The verification of the obtained numerical results has been performed using the less economic Muller boundary IE. It has shown that the model of compensated GBC with Nystrom-type discretization allows obtaining reliable data with small errors in the range from 1.5% to 4%.

In the case of H-polarization, we have investigated the transversal resonances. At the corresponding frequencies the strip is almost transparent for a normally incident plane wave, thus only the edges of the strip scatter. The spectral dependences of the total scattering cross-sections and absorption cross-sections for the strip with $\varepsilon_r = 1000 + i$ (see. Fig. 1(a)) have demonstrated the most dramatic resonance peak around $\kappa \approx 20$ accompanied by a jump in the absorbed power by 2 orders of magnitude and a drop in the backscattered power by almost 3 orders of magnitude. This is the frequency at which

the thickness of the material slab equals half-wavelength in material, $k_0 h |\varepsilon_r|^{1/2} \approx \pi$. In addition, we have also investigated the case of the edge-on incidence. In this situation, the dielectric strip remains "visible" even in the case of H-polarization as it still scatter and absorb light in contrast to the zero-thickness PEC strips which are "invisible".

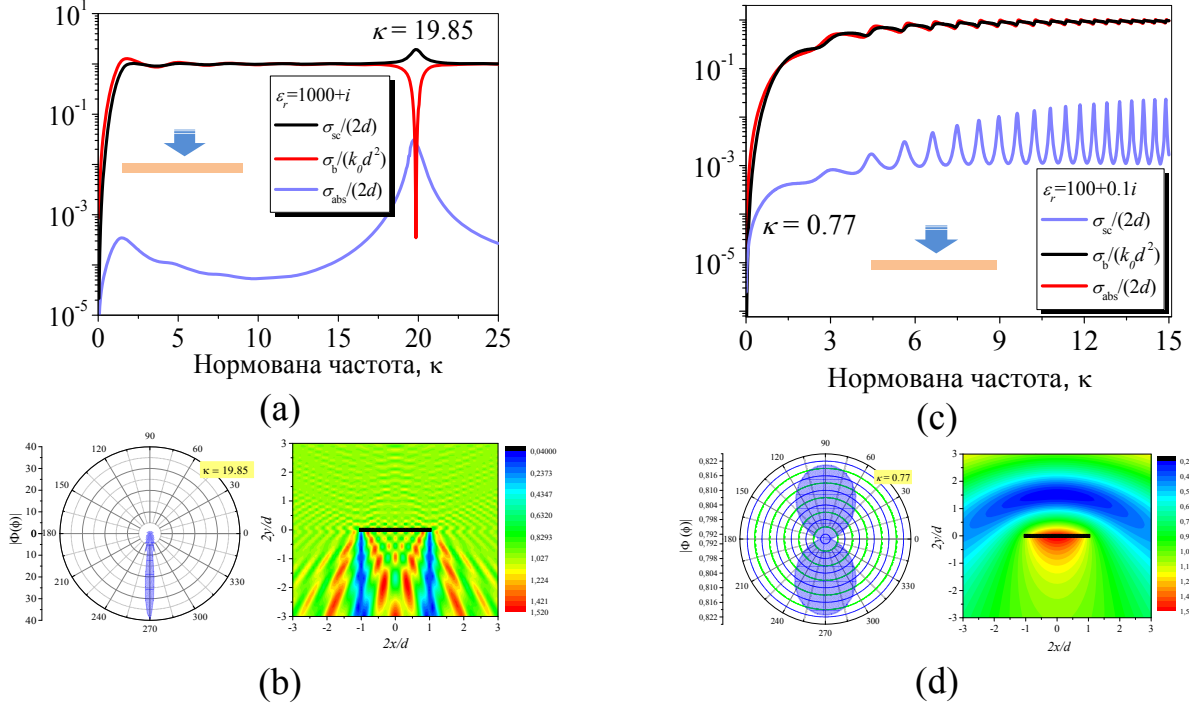


Figure 1. (a) Normalized total scattering cross-section (black), absorption cross-section (blue) and backscattering cross-section (red) as a function of the normalized frequency for dielectric strip $\varepsilon_r = 1000 + i$ (H-polarization case). (b) The scattered far-field and total near-field patterns at $\kappa = 19.785$. (c) and (d) The same as in panels (a) and (b) however in the E-polarization case for $\varepsilon_r = 100 + 0.1i$ at $\kappa = 0.77$ (in the E_{10} resonance).

In the case of the E-polarization, both the scattering and the absorption spectra demonstrate a sequence of resonances. They are explained as the longitudinal Fabry-Perot resonances, $E_{p0}, p=1,2,3,4,\dots$, on the natural guided wave of the corresponding dielectric layer traveling from one end of the thin strip to another (see Fig. 1(c)). Such effects are weakly observed in the H-polarization case because the propagation constant of the natural wave of the corresponding dielectric layer is very close to the free-space wavenumber (see Fig. 1(a)).

The third chapter deals with 2-D scattering problems for the H- and E-polarized electromagnetic plane waves incident on a thin stand-alone noble-metal nanostrip (of silver or gold) in the optical range, and also on a finite grating $S = \bigcup_{j=1}^N S_j$ consisting of

N parallel nanostrips $S_j = \{(x, y) : (j-1)p \leq x \leq (j-1)p + d, -h/2 \leq y \leq h/2\}$ of permittivity $\varepsilon_r(\lambda)$, width d , thickness h and period p (see Figs. 2 and 3). To characterize the complex dielectric permittivity of silver or gold we take the experimental data of Johnson and Christy and use Akima cubic-spline interpolation scheme to eliminate the wiggles in the interpolant

Further, keeping in mind that $h \ll \lambda$ in the visible range, we neglect the internal fields inside each of the strips and impose the two-side GBCs (1) for the external field limiting values at $L = \bigcup_{j=1}^N L_j$, where $L_j = \{(x, y) : (j-1)p \leq x \leq (j-1)p + d, y = 0\}$ is the median line of the j -th strip. Herewith the scattered field is sought in the form of

$$U^{sc}(\vec{r}) = k_0 \sum_{j=1}^N \int_{L_j} v_j(\vec{r}') G(\vec{r}, \vec{r}') d\vec{r}' + \sum_{j=1}^N \int_{L_j} w_j(\vec{r}') \frac{G(\vec{r}, \vec{r}')}{\partial \vec{n}(\vec{r}')} d\vec{r}', \quad (8)$$

where $v_j(\vec{r})$, $w_j(\vec{r})$, $j = 1, 2, \dots, N$ are unknown effective electric and magnetic surface currents induced by the incident field on the S_j -th strip. Finally, a discrete model of the H- and E-polarized electromagnetic plane wave scattering by finite strip gratings has been built. It has the form of two independent sets of singular and hyper-singular IEs for unknown functions $v_j(\vec{r})$ and $w_j(\vec{r})$, $j = 1, 2, \dots, N$, respectively. For the discretization of the obtained sets of the IEs we use the mentioned above Nystrom-type method with the quadrature formulas of interpolation type adapted to the edge behavior.

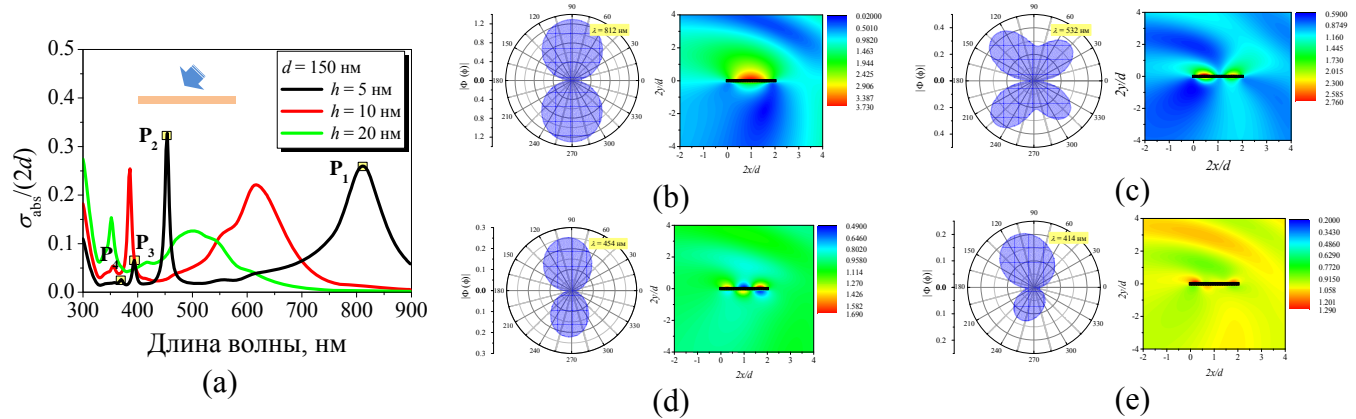


Figure 2 – (a) Normalized total scattering cross-section as a function of the wavelength. The scattered far-field and total near-field patterns in plasmon resonances at $\lambda_{P1} = 812$ nm (b), $\lambda_{P2} = 532$ nm (c), $\lambda_{P3} = 454$ nm (d), and $\lambda_{P4} = 414$ nm (e) (H-polarization case).

The numerical investigation of the actual rate of the Nystrom-type method convergence has been carried out. It has been found that the order of interpolation polynomial approximating the surface current on each strip for all $j = 1, 2, \dots, N$ does not depend on the general dimensions of the grating, as far as they are separated with gaps

larger than several nanometers. Thus, for the grating consisting of 200 strips with period of 600 nm (which corresponds to the grating of total width of 600λ in the optical range), to achieve 4-digit accuracy in the analysis one can take $n_v = n_w = 50$. At the same time, the orders of the corresponding full matrices, obviously, equal $N \times n_{w,v}$.

In the case of H-polarization we have investigated both the regularities and the specific features of the surface plasmon resonances on the noble-metal nanostrips in the optical range and on finite flat gratings of them. These resonances are the Fabry-Perot-like resonances H_{p0} , $p=1,2,3,4,\dots$ on the delocalized “short-range” surface plasmon wave of a silver slab traveling between the strip edges.

It has been shown that the surface plasmon excitation leads to a marked enhancement of the scattering and absorption. It has been also demonstrated that intensity and position of the plasmon resonances depend on the geometrical parameters such as nanostrip width and thickness and on the strip material. This, in its turn, allows tuning of the surface plasmon resonances and reaching more efficient light scattering and/or absorption by varying the geometrical and material parameters of the strip.

In Fig. 2, we present the normalized (by the number of strips N) total scattering cross-section as a function of the wavelength for the strips of fixed width $d = 150$ nm and thickness values of $h = 5, 10$ and 20 nm, under the inclined incidence ($\beta = \pi/4$) of the H-polarized plane wave. The portraits of the total magnetic field in the near zone and the corresponding far-field patterns in the first four plasmon resonances are presented in Fig. 2 (b)-(e) for the silver strip with parameters $d = 150$ nm and $h = 5$ nm.

Besides, it has been found that the absorption cross-section can serve as a better than total scattering cross-section figure-of-merit for visualizing the higher-order plasmon resonances. Note that the even-index resonances can be excited only at the inclined incidence because of their modal field anti-symmetry across the y -axis.

It has been found that, in the case of the H-polarized plane wave scattering by a finite flat grating of noble-metal nanostrips, two type of the resonances are excited: surface plasmon resonances and specific grating resonances caused by the periodicity (so-called, geometrical, collective, or lattice resonances). More broadly, these resonances display a variety of asymmetric Fano shapes near so-called Rayleigh anomalies of associated infinite gratings, at $\lambda_{G_m} = \lambda_m^{R.A.} + \delta_m$, where $\lambda_m^{R.A.} = (\cos \beta \pm 1)p / m$ for all $m = 1, 2, \dots$. Fig. 3(a) demonstrates a comparison of the optical responses of finite gratings consisting of $N = 50, 100$ and 200 silver strips with parameters $d = 250$ nm, $h = 20$ nm and $p = 450$ nm. As one can see, in the vicinity of the grating resonance, at $\lambda_{G_1} = 452$ nm, the magnetic field has the form of standing wave formed by two ± 1 -st Floquet harmonics propagating along the grating. It has been shown that Q-factors of the grating resonances strongly depend on the overall grating dimensions such as width, thickness and strip number, while their wavelengths quickly tend to the exact values of the associated Rayleigh anomalies for $N = \infty$. In addition, we have investigated the mutual influence of the plasmon resonances and the resonances on the grating modes.

It is well known that in the case of the E-polarization an infinite metal layer does not support guided surface-plasmon waves, in the visible. As a result, stand-alone metal strips or finite gratings of such strips do not support localized surface plasmon resonances.

At the same time, in contrast to the H-polarization, finite strip gratings demonstrate a gradual build-up of the Rayleigh anomalies as the strip number gets larger; this takes form of suppression of both the scattering and the absorption in the vicinity of the associated Rayleigh anomalies. As we have found, this is because at these wavelengths the strips happen to be located in the deep minima of the electric field.

For completeness, a comparison of the optical properties of finite and infinite flat silver-strip gratings has been performed. This requires an adequate common figure-of-merit to be selected that is not an obvious matter. However, we have found that the reflectance of a plane wave by a finite grating can be introduced as the part of TSCS associated with the power scattered into the upper half-space. The transmittance of finite grating can be introduced in similar manner however with account of the optical theorem. Thus, in terms of such defined coefficients of the reflectance, transmittance and absorbance the role of the number periods in the formation of the optical properties of the strip grating has been demonstrated.

Finally, the sensitivities of the optical resonances of the finite silver strip gratings have been studied. By the example of a stand-alone silver strip it has been shown that the higher order plasmons exhibit much higher bulk refractive-index sensitivities. At the same time, due to the higher Q-factor, the 2nd order surface plasmon P_2 demonstrates the value of the figure-of-merit (FOM) 5.5 times higher than that of the primary plasmon P_1 .

The fourth chapter deals with 2-D scattering problems for the H- and E-polarized electromagnetic plane waves and finite comb-like strip gratings consisting of N identical strips $S_j = \{(x, y) : x \in [(j-1)p - h/2, (j-1)p + h/2], y \in [0, d]\}$ (Fig. 4).

The main difference of the comb-like grating from the flat one is that "area" of the latter grating is not infinitely thin.

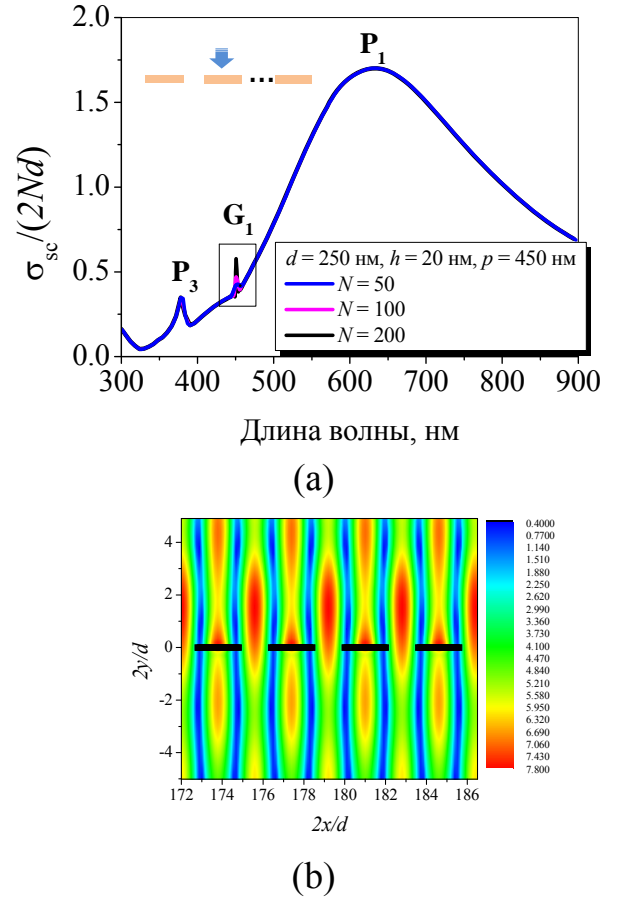


Figure 3 – (a) Normalized total scattering cross-section as a function of the wavelength.
(b) Total near-field pattern in the grating resonance at $\lambda_G = 452$ nm.

This, in its turn, leads to a coupled set of singular and hyper-singular IEs for unknown surface currents $v_j(\cdot)$ and $w_j(\cdot)$. However, the properties of the kernels of the obtained IEs are the same as for a flat grating. Thus, as a reliable instrument for the solving such IEs, the same Nystrom-type method based on the quadrature formulas of interpolation type with guaranteed convergence and controlled accuracy of computations can be successfully used.

In all, three different types of optical resonances have been observed and analyzed in the scattering of an H-polarized plane wave by a finite comb-like silver-strip grating: localized surface plasmon resonances on strips, “cavity” resonances (or “gap” resonances) between adjacent strips, and periodicity-induced grating resonances in the vicinity of the corresponding Rayleigh anomalies. In Fig. 4(a), we present the data on the normalized total scattering cross-sections under the H-polarized plane wave incidence for the grating consisting of $N = 1, 2, 10, 20, 50$ and 100 silver strips with parameters $d = 300$ nm, $h = 20$ nm and $p = 500$ nm. As one can see, for a stand-alone 300×50 nm² silver strip ($N = 1$), two plasmon modes of the 1st and 2nd orders are observed in the visible band (black curve) at the resonance wavelengths $\lambda_{p1} = 697.5$ nm and $\lambda_{p2} = 413.2$ nm. If the strips are two ($N = 2$), the scattering spectrum keeps certain features characteristic for the single strip: the 2nd order plasmon resonance is only slightly deformed and the 1st order plasmon resonance becomes less visible (twice lower in amplitude) because of the shadowing of the left strip by the right one. Still the spectra for $N = 2$ display something new: a strong resonance peak at the wavelength of $\lambda = 507$ nm. This new feature is kept almost intact if the number N is taken larger.

It allows to conclude that this resonance is associated with the so-called “cavity mode” or “gap plasmon” mode. Thereby, if $N = 2$, the grating can be viewed as an open two-mirror Fabry-Perot resonator. If $N > 2$, we have a system consisting of $N - 1$ coupled Fabry-Perot resonators and, as a result, a strong optical interaction between adjacent strips which leads to the excitation of the high-quality cavity resonance. This interpretation is supported by the fact that the wavelength and the quality factor of the

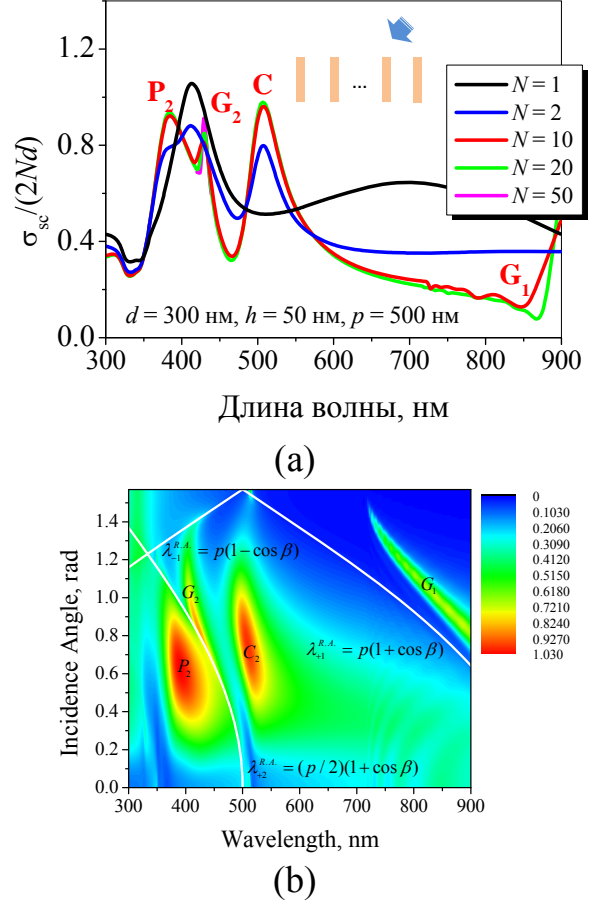


Figure 4 – (a) Normalized total scattering cross-section as a function of the wavelength. (b) Relief of the total scattering cross-section as a function of the wavelength and incidence angle.

cavity resonance are almost independent of the number of strips if $N > 2$. At the same time, the Q-factor of the grating resonance of the comb-like strip grating is tens times higher than the same value of the corresponding finite flat strip grating. Besides, it has been shown that the interplay between plasmons, resonances on the grating and the cavity modes depends on the angle of incidence, period of the grating, and the width and thickness of each strip. Choosing these parameters in optimal manner may help design periodic nanosensors, absorbers, and SERS substrates with improved characteristics.

Similarly to flat gratings of strips, it has been demonstrated that the E -polarized plane wave scattering by the finite comb-like strip gratings does not excite surface plasmon resonances in the optical range.

However, in the case of normal incidence in the vicinity of the Rayleigh anomalies it has been observed a pronounced suppression of both the scattering and the absorption. Besides, under the edge-on incidence on the grating, the optical interaction between the adjacent strips induce intensive cavity resonances, appearing in far zone as Bragg effects at the wavelengths satisfying the Bragg law, $2p \cos \beta = \lambda m$, $m = 1, 2, \dots$

Finally, the bulk sensitivity and the FOM values of optical resonances on finite comb-like silver strip gratings have been studied. It has been shown that resonances on the cavity modes are more sensitive to the refractive-index changes than those on plasmons. At the same time it has been found that the bulk sensitivity of the grating resonances is proportional to the period and does not depend on the refractive index of the host medium. These resonances exhibit much higher values of both the bulk refractive-index sensitivities and FOM than the optical resonances on surface plasmons.

Thus, the mentioned optical resonances of the finite comb-like strip gratings have high potential for the use in sensing applications in the visible and near-infrared ranges and are promising for the design of new optical biosensors with modified characteristics.

The fifth chapter is dedicated to the analysis of 2-D H- and E-polarized plane wave scattering problems associated with flat gratings consisting of finite number N of identical graphene strips $S_j = \{(x, 0) : (j-1)p \leq x \leq (j-1)p + d\}$, $j = 1, \dots, N$ in the THz frequency range. Each of these problems is reduced to a set of either the Fredholm IEs of the second kind or hyper-singular IEs depending on the polarization (see Fig. 4).

Graphene monolayers are electrically infinitesimal thin (single-atom) layers and display rather good electron conductivity $\sigma(\omega, \mu_c, \gamma, T)$ that mainly depends on frequency ω , temperature T , electron relaxation time τ , and chemical doping μ_c . In addition, one of the most promising features of graphene as compared with metals is the opportunity to modify its conductivity by applying an external electrostatic biasing field, which modifies graphene chemical potential. This can be easily implemented, for instance, by including an extremely thin polysilicon layer below the dielectric which supports graphene, and applying a DC bias between these two layers. Graphene is very interesting in view of possibility of strong interaction with electromagnetic waves in the THz frequency range. Indeed, it is able to support delocalized surface-plasmon waves at frequencies two orders of magnitude lower than the noble metals.

The complex-valued graphene conductivity is calculated via Kubo's formalism. The graphene monolayer can be electromagnetically characterized with the aid of the following resistive boundary conditions on a zero-thickness boundary with electric complex resistivity (surface resistance), $R = 1 / (\sigma Z_0)$,

$$[\vec{E}_{tg}^+ + \vec{E}_{tg}^-] = 2\sigma^{-1}\vec{n} \times [\vec{H}_{tg}^+ - \vec{H}_{tg}^-], \quad \vec{E}_{tg}^+ = \vec{E}_{tg}^-, \quad (9)$$

imposed on the limiting values of the field components tangential (tg) to the top (+) and bottom (-) sides of the layer.

As we have found, a stand-alone microsize graphene strip and corresponding finite strip gratings illuminated by the H-polarized waves in the THz frequency range demonstrate a variety of surface-plasmon resonances of asymmetric Fano shapes at much lower frequencies than in the case of the noble-metal strips. It has been shown that the magnitudes of the surface-plasmon resonances are quite sensitive to the relaxation time changes. The peaks on the scattering and absorption spectra became more pronounced if τ increases due to the smaller dissipation losses. Moreover, it is observed that an increase of the chemical potential μ_c leads to the lower losses and an up-shift of the frequencies where graphene presents large inductive behavior. In addition, it has been shown that in the H-polarization case finite graphene-strip gratings do not exhibit grating resonances which were found for finite noble-metal strip gratings. This is explained by the 2-D nature of graphene as a single-atom layer and thereby the absence of the effective magnetic currents on the graphene strips. Still in both the H- and the E-polarization cases we have found a suppression of the scattering and absorption in the vicinity of the associated Rayleigh anomalies, more pronounced in the E-case.

Finally, the bulk refractive-index sensitivities and FOM values of the plasmon resonances on a stand-alone micro-size graphene strip have been calculated. It has been found that the primary plasmon mode P_1 is more sensitive ($60 \mu\text{m}/\text{RIU}$) to the refractive-index changes than plasmons of the higher orders – P_3 ($22.8 \mu\text{m}/\text{RIU}$) and P_5 ($14.5 \mu\text{m}/\text{RIU}$). However, the last ones demonstrate much higher FOM values explained by the higher Q-factors.

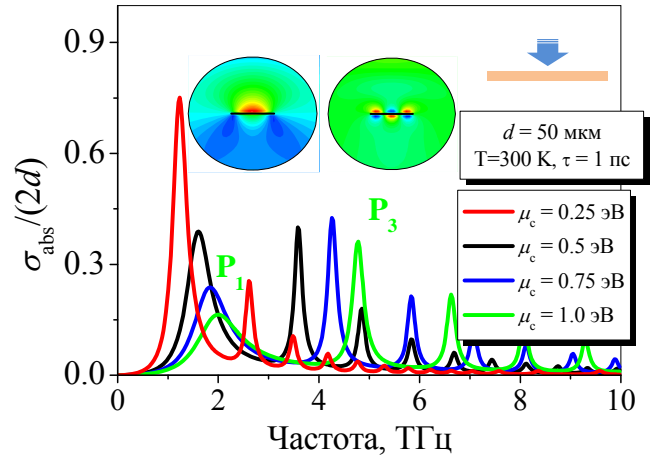


Figure 4 – Normalized total scattering cross-section as a function of the frequency. In the inset, total near-field patterns of the first plasmons at $f_{P1} = 2.06$ THz and $f_{P3} = 4.83$ THz.

CONCLUSIONS

In the thesis, an important problem of today's electromagnetics has been solved: an efficient numerical method has been developed to study both the regularities and the specific features (resonances) in the scattering and absorption of electromagnetic waves by finite material thin-strip gratings (dielectric, noble-metal in the optical range, and graphene in the THz range). It is based on the model combining the two-side GBC or resistive-sheet boundary conditions (with complex-valued resistivities) and a Nystrom-type method using the quadrature formulas of interpolation type for the discretization of the associated logarithmically-singular and hyper-singular IEs. Besides, we have performed numerical analysis, with guaranteed convergence and controlled accuracy of computations, of the scattering and absorption characteristics of various finite strip gratings as bulk refractive-index sensors.

The main scientific and practical results are as follows:

- A mathematically grounded 2-D model of the H- and E-polarized electromagnetic plane wave scattering by a finite thin-strip grating (dielectric, noble-metal in the optical range and graphene in the THz range) has been built. The model is based on the boundary-value problem for Maxwell's equations with two-side GBC or resistive boundary conditions, radiation condition, and local finiteness of energy. Using the a priori known behavior of the surface currents at the strip edges we have reduced each problem to an equivalent set of singular and hyper-singular IEs;
- Novel numerical algorithm for solving the sets of singular and hyper-singular IEs has been developed. It is based on the Nystrom-type discretization with the aid of the quadrature formulas of interpolation type which guarantee convergence and controlled accuracy of computations;
- The advantages of the developed numerical method and the proposed model have been demonstrated, as well as full agreement of the obtained numerical results with those obtained with known commercial computer-aided-design codes;
- Physical regularities of the influence of geometrical and material parameters (width, thickness, grating period and strip number) on the scattering and absorption characteristics have been studied;
- The nature and specific features of the localized surface plasmon resonances of the primary and higher orders have been investigated for the gratings consisting of finite number of noble-metal nanostrips in the optical range and micro-size graphene strips in the THz range;
- The grating resonances induced by the periodicity have been found in the scattering and absorption of the H-polarized plane waves by the finite grating consisting of thin noble-metal strips. Their properties in dependence on the geometrical and material parameters of gratings have been investigated for the first time;
- Mutual influence of the localized surface plasmons and the resonances on the grating modes has been revealed;

- It has been demonstrated that the Q-factors of the grating resonances on the comb-like finite strip gratings can be tens times higher than Q-factors of the grating resonances of the corresponding flat finite strip gratings;
- The bulk refractive-index sensitivities of the optical resonances on comb-like finite silver nanostrip gratings have been studied for the first time.

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