National Academy of Sciences of Ukraine
O. Y. Usikov Institute of Radio-Physics and Electronics

Denys M. Natarov

PLASMON AND GRATING MODES IN THE SCATTERING, ABSORPTION, AND EMISSION OF OPTICAL WAVES BY FINITE NANOWIRE GRATINGS

01.04.03 – Radio Physics

Abstract
of the thesis submitted in the partial fulfillment of the
Ph.D. degree requirements in Physics and Mathematics

Kharkiv, Ukraine - 2019

Academic Supervisor:	Alexander I. Nosich D.Sc., Professor, Head of Laboratory of Micro and Nano Optics O. Y. Usikov Institute for Radio-Physics and Electronics NASU Kharkiv, Ukraine
Official Reviewers:	Mykola G. Kokodiy D.Sc. Professor, Department of Physics National University of Pharmacy, Kharkiv, Ukraine
	Volodymyr M. Fitio D.Sc. Professor, Department of Photonics Lviv National Polytechnic University, Lviv, Ukraine

Public defense will take place on April 4, 2019 at the session of the Specialized Jury in Radio Physics # Д 64.157.01 in the O. Y. Usikov Institute of Radio-Physics and Electronics of the National Academy of Sciences of Ukraine. Address: IRE NASU, vul. Proskury 12, Kharkiv 61085.

The thesis is available for reading at the scientific library of IRE NASU, vul. Proskury 12, Kharkiv 61085.

This Summary was released on March 2, 2019

Scientific secretary of the Specialized Jury — I.V. Ivanchenko

GENERAL DESCRIPTION

This thesis is dedicated to the analysis of scattering and absorption of light by finite gratings of various forms made of nanosize dielectric and silver wires, as well as the analysis of eigenmodes, their frequencies and self-excitation thresholds for such gratings as finite-periodic open resonators. The analysis is performed using the boundary value problems for the linear time-harmonic Maxwell equations, which are reduced to the Fredholm second kind matrix equations.

Timeliness of research. General trend in the development of electromagnetic-wave science and technology is mastering the shorter-wave ranges, in particular, terahertz, infrared and visible-light ones. The development of nanotechnologies has already allowed controllable creation of gratings made of objects that are smaller than the wavelengths even in the visible range. Besides, nanoscale materials and devices have given impetus to the development of new areas such as nanophotonics and nanooptics. Resonance phenomena in the scattering and absorption of visible light by metallic nanoscale objects are mainly due to the excitation of surface plasmon resonances, and have a wide range of practical applications. For example, when developing biosensors, plasmon effects can significantly enhance the detection and identification capabilities of biological substances in small concentrations.

Thanks to the modern technologies of molecular beam epitaxy, deposition and etching, thin nanowires and nanostrips made of dielectrics and noble metals have firmly been included in many devices of the terahertz and visible light wavelength ranges, for example, nanoantennas and biosensors. At the same time, periodic structures, that is, gratings of nanowires and nanostrips are especially attractive. This is due to the recently discovered effects of abnormal reflection, transition, absorption and emission of light, as well as the giant effects of Faraday, Kerr, Kerker, nonlinear generation of the second harmonic, and others. In general, such phenomena have the form of Fano-type resonances and are observed near the Rayleigh anomalies of the corresponding infinite gratings. At present, the theoretical study of these phenomena on the models of infinite gratings has shown that they appear due to the existence of specific high-quality modes, called grating (a.k.a. lattice) modes. They were studied, in particular, in the works of V. O. Byelobrov, T. L. Zinenko, O. V. Shapoval and A. I. Nosich. It is important to note that a systematic study of the grating modes of finite gratings of circular nanowires has not been performed before.

In this work, the scattering and absorption properties of the gratings consisting of tens and hundreds of nanowires are studied. As a reliable computational tool, we use the well-known classical expansion of the field function in terms of the Fourier series in azimuth exponents in the local polar coordinates of each wire. Using the addition theorems for cylindrical functions and applying the boundary conditions on the surface of each wire, we obtain a finite-block matrix equation, where each block is infinite. However, in contrast to most of the works that used this method, in order to ensure that the solution has a guaranteed convergence, in this work the unknown coefficients are renormalized in such a way that the infinite matrix equation becomes a Fredholm second kind equation. Then each of its blocks can be truncated to a finite size, and the larger this size, the closer the solution to the exact one.

Recently, a new direction in nanophotonics research related to the plasmon modes has been developing rapidly: the analysis and development of plasmonic nanolasers, where nanosize metal particles or wires, strips and tubes are open nanoresonators, and the active zone is introduced in various ways. In this dissertation the properties of eigenmodes of circular silver nanowires and nanotubes, as well as gratings of them, are considered. The performed here analysis of laser modes uses the lasing eigenvalue problem (LEP), which was introduced in the early 2000's in the works of E. I. Smotrova and A. I. Nosich. This approach allows finding the lasing modes, their frequencies and self-excitation (i.e. steady radiation) thresholds using the apparatus of classical electromagnetics. Besides of the plasmon modes, we also find grating modes of nanolasers based on nanowire gratings; such modes have low self-excitation thresholds that are very attractive to developers of such devices.

Relationship with scientific programs, plans and themes. This work has been performed in the Laboratory of Micro and Nano Optics of the Quasioptics Department of IRE NASU, in the framework of the following projects:

1. Competitive research project of the Ministry of Education and Science, Ukraine «Innovative numerical simulation of quasioptical focusing systems» (#0109U005351, 2009-2010).
2. National Target Program "Nanotechnologies and Nanomaterials": project «Fundamental mathematical and numerical studies of optical electromagnetic fields of stand-alone and coupled microcavity lasers with nanosize active regions shaped as layers, wires and strips» (#0110U004737 2010 -2014).
3. Research project of NASU: «Development of methods of optics and quasioptics for establishing the regularities and peculiarities of the interaction of terahertz radiation with physical and biological objects» (#0111U001079, 2012-2016).
4. Research project of NASU: «Development and application of optical and quasioptical methods for studying the processes of generation and transformation of electromagnetic waves of the terahertz, infrared and visible ranges» (#0117U004036, 2017-2019).
5. Scientific exchange program between NASU and the Turkish National Committee for Scientific and Technical Research, joint project with Bilkent University, Ankara «Innovative electromagnetic modeling of multi-element quasioptical focusing systems of the millimeter-wave and terahertz ranges», (#106E209, 2007-2009).
6. Research and Networking Program of the European Science Foundation «Newfocus: New frontiers in millimeter and sub-millimeter wave integrated dielectric focusing systems», project «Resonances in the scattering and focusing of waves by periodically structured ensembles of metal and dielectric wires» with the Institute of Electronics and Telecommunications of the University of Rennes 1, France (2010).

7. Program of the European Science Foundation «Plasmon-Bionanosense: New approaches to biochemical sensing with plasmonic nanobiophotonics», project «Modes of core-shell nanowire and nanotube plasmonic lasers» with the Institute of Photonics and Electronics of AS of Czech Republic, Prague (2015).

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

- «Resonant scattering of electromagnetic waves by finite periodic configurations of sub-wavelength circular wires», IEEE AP-S Pre-Doctoral Award, 2011.
- «Broadband resonance absorption and scattering of light for ultrathin plasmonic solar cells and biosensors: modelling and optimization», International Visegrad Fund, with the Institute of Telecommunications, Warsaw, Poland, 2012-2013.
- «Plasmon and periodicity assisted wideband absorbers for solar cells and biosensors», Rennes Metropole Mobility Grant with the Institute of Electronics and Telecommunications of the University of Rennes 1, France, 2013.

Research goals and tasks. The goal of the research, firstly, is to study the features and regularities of the scattering of plane electromagnetic waves by finite gratings (one-periodic and two-periodic, in the form of discrete corner, cross, parabolic reflector, in a "cloud" with arbitrary located wires) made of dielectric or silver nanowires of circular cross-section in the optical wavelength range, and secondly, to study the eigenmodes of nanolasers based on silver nanowires and nanotubes with active shell and core (for the tube) and based on finite number of quantum (i.e. active) nanowires and silver nanowires with active shells.

In the first case, the scattering and absorption of plane waves of two polarizations are considered; their features are studied when changing the grating parameters. In the second case, we are looking for eigenfields of the lasing modes of the studied structures, and their emission frequencies and self-excitation thresholds, focusing on the regularities and features of their dynamics studied when changing the parameters of the wires, tubes and gratings of them.

In order to achieve these goals, the following tasks were considered:

- construction of two-dimensional (2-D) mathematical model, based on the analytical regularization, of the scattering of H- and E-polarized plane waves on an arbitrary ensemble made of finite number of parallel dielectric or silver wires of circular cross-section;
- development of convergent numerical algorithms for calculating the scattering and absorption characteristics, as well as the fields in the near and far zones of the studied structures;
- systematic calculation of the characteristics of resonance scattering and absorption of waves, as well as resonance fields in the near and far zones;
- development of numerical algorithms for solving the LEP problems for nanolasers based on single silver wire and silver tube with an active zone and gratings of finite number of quantum or silver wires;

- systematic calculation of eigenfields, frequencies and self-excitation thresholds of modes of such nanolasers.

The object of research is the phenomena of the scattering and absorption of plane electromagnetic waves by finite periodic gratings of circular material nanowires, as well as the emission of electromagnetic waves by open resonators based on nanowires and gratings of them, equipped with active regions.

The subject of the study is the resonance characteristics of the scattering and absorption of waves by finite periodic gratings of circular material nanowires, as well as the eigenmodes of such gratings, that is, the spectra of frequencies and self-excitation thresholds of lasing modes of open resonators based on nanowires and finite gratings of them, along with their eigenfields.

Research methods. In this work, the methods of the theory of boundary-value problems of classical electromagnetics are used. Every problem of the scattering of waves is formulated as a boundary value problem for a field function which satisfies the Maxwell equations with exact boundary conditions, the condition of radiation at infinity, and the condition of the local power finiteness. Using the partial separation of variables and the addition theorems for cylindrical functions, the finding of the field Fourier coefficients is reduced to a Fredholm second kind matrix equation with finite number of blocks corresponding to the number of wires. Each block of such equation is infinite and truncated to finite number N, and the convergence to the exact solution with a growth of N is guaranteed. The lasing eigenvalue problem is stated with the same conditions but in the absence of the incident field, and the mode frequencies and self-excitation thresholds of lasing are found with controlled precision as the roots of the corresponding determinant equation.

Scientific novelty of obtained results

- in the scattering of H-polarized waves by finite gratings of circular dielectric nanowires, the grating resonances were studied first time;
- in scattering and absorption of H-polarized electromagnetic waves by finite gratings of circular metal nanowires in the light range, two types of resonances have been demonstrated: on plasmon and grating modes; their interactions and the influence of geometric and material parameters on the scattering and absorption characteristics were studied first time;
- electromagnetically-induced transparency was demonstrated for the first time in the scattering characteristics of the latter gratings when the plasmon and grating resonances overlap;
- for the first time, a comparative analysis of the coefficients of reflection from finite gratings of metal nanowires and corresponding infinite ones was done; it was concluded that near to the frequencies of the grating resonances, to have the reflection coefficients close to each other, much more wires are needed (not less than 100) than off that range (about 10);

- the ability to focus light waves with discrete parabolic reflectors of metal nanowires was studied if the plasmon resonance is excited on each of the wires; in contrast, grating resonances were shown to produce no focusing;
- for the first time, a "signature of periodicity" was analyzed; it appears on the reliefs of the total scattering cross-section as a function of the wavelength and the angle of incidence in the presence of a periodic chain of nanowires in a "cloud" of arbitrary located nanowires;
- for the first time, the eigenmodes were found and classified of nanolasers based on silver nanowires and nanotubes with active shell and core; the effect of geometrical parameters on the frequency and self-excitation thresholds was studied;
- for the first time, the grating modes of finite number of dielectric or silver nanowires with low self-excitation thresholds were found and the influence of geometric and material parameters on their frequency and self-excitation thresholds was studied.

Practical value of obtained results. The method used in this work and numerical algorithms developed on its basis can be applied to analyze, with prescribed accuracy, the scattering and absorption characteristics of electromagnetic waves, the near and far fields, as well as the frequencies and self-excitation thresholds of lasing modes of arbitrary ensembles of finite number of circular material wires of arbitrary radius.

The obtained results of numerical analysis of the characteristics of scattering and absorption of light waves by various gratings of circular nanowires expand our knowledge and have fundamental significance. Besides, they have practical impact as the gratings of metal and dielectric sub-wavelength wires are widely used in the design of antennas, sensors, absorbers of solar panels, etc.

The analysis of the plasmonic modes of nanolasers based on single silver nanowires and nanotubes, as well as gratings of nanowires, and the grating modes of the latter, can help in the creation of new, more efficient nanolasers with low self-excitation thresholds.

Personal contribution of the author. The main results presented in the dissertation were obtained the author. In the co-authored works [1-4,6-9] his contribution consists in the derivation of the basic equations, the development of numerical algorithms, the writing of the corresponding code, as well as in the systematic calculation of the scattering and absorption characteristics, the scattering angular patterns and the near fields for the gratings of finite number of nanowires, together with the interpretation of the obtained results.

Dissemination of results. The results of the work were discussed and reported at the following scientific seminars: IRE NASU (Prof. P. M. Melezhyk), George Green Institute for Electromagnetics Research of the Nottingham University, UK (Prof. T. M. Benson), Institute of Telecommunications, Warsaw, Poland (Prof. M. Marciniak), Institute of Photonics and Electronics AS Czech Republic, Prague (Prof.

J. Chtyroki), Nihon University, Japan (Prof. T. Yamasaki), and Tokyo Institute of Technology, Japan (Prof. M. Ando). In addition, they were presented at the following international conferences, workshops and symposia:

- International Conference on Transparent Optical Networks (ICTON), Munich (2010), Stockholm (2011), Cartagena (2013),
- International Symposium on Physics and Engineering of Microwaves, Millimeter and Sub-Millimeter Waves (MSMW), Kharkiv (2010, 2013)
- Asia-Pacific Radio Science Conference (AP-RASC), Toyama (2010),
- IEEE Conference on Mathematical Methods in Electromagnetic Theory (MMET), Kyiv (2010, 2018), Kharkiv (2012), Lviv (2016),
- International Conference on Theoretical and Computational Nanophotonics (TACONA), Bad Honnef (2011),
- European Conference on Antennas and Propagation (EuCAP), Prague (2012),
- International Conference on Near-Field Optics (NFO), San Sebastian (2012),
- International Symposium on Antennas and Propagation (ISAP), Nagoya (2012),
- IEEE Conference on Electronics and Nanotechnoljgy (ELNANO), Kyiv (2013, 2014, 2015),
- International Conference on Microwaves, Radar and Wireless Commmunications (MIKON), Gdansk (2014),
- URSI General Assembly and Scientific Symposium (URSI-GASS), Beijing (2014),
- IEEE Conference on Advanced Optoelectronics and Lasers (CAOL-LFNM), Sebastopol (2010), Kharkiv (2011), Sudak (2013), Odesa (2016),
- Young Scientist Forum on Applied Physics (YSF), Kharkiv (2016),
- IEEE First Ukraine Conference UKRCON, Kyiv (2017),
- International Workshop on Direct and Inverse Problems of Electromagnetic and Acoustic Wave Theory (DIPED), Tbilisi (2018).

Publications. The results of research were published in 37 refereed papers, including 7 papers in scientific journals [1-7] and 30 papers in the proceedings of international conferences, the main of which are [8-13].

Structure and volume of thesis. The thesis includes Introduction, 4 chapters, Conclusions, and List of References. Total size of thesis amounts 187 pages, from which 17 pages are for the list of references.

THESIS CONTENT

Introduction grounds the timeliness of the chosen topic of the thesis, formulates the goals and tasks of research, and gives its general data.

Chapter 1 is devoted to an overview of literature around the topic of the dissertation, i.e. the studies of the scattering of electromagnetic waves by finite gratings of circular wires. Several of the most common methods for analyzing this problem are explained, as well as their disadvantages and limitations. Next presented is a general summary of the plasmonic resonance effects observed in the light scattering by metal particles. Also, the wavelength dependences of the real and imaginary parts of the dielectric function of silver in the visible range, which are calculated using several analytical models based on the Drude formula, as well as the experimental data of Johnson and Christi, approximated by splines, are also given. His is followed by a description of the existence of grating modes (GM) in periodic structures. The characteristics of scattering and absorption which are used in the work are presented, as well as an optical theorem, which connects the total scattering (TSCS) and absorption cross-sections (ACS), the sum of which is the extinction, to the forward scattering amplitude in the far zone. Then the lasing eigenvalue problem is formulated and explained, tailored for the analysis of the eigenmodes of nanolasers as metal-dielectric open resonators with active regions.

In Chapter 2, the problem of the scattering and absorption of the visible light waves by a linear grating of a finite number of nanowires is studied. The cross-section of such a grating is shown in Fig. 1. First of all, a generic two-dimensional (2-D) problem of the scattering of the E- or H-polarized plane wave by M parallel wires of circular cross-section is considered. It is treated by expanding the field function, which satisfies the 2-D Helmholtz equation with coefficient $k^2\alpha^2$ inside each wire (where k is the wavenumber and α is the complex refractive index of the wire material) and k^2 outside, in terms of the Fourier series in each of the regions in the local azimuth coordinate of each wire, with taking into account Sommerfeld radiation condition and condition of the local power finiteness. After applying of boundary conditions, which consist in the continuity of the tangential field components on the boundary of each wire, the problem is reduced to a matrix equation built of $M \times M$ blocks, each being infinite, for the vector of unknown field expansion coefficients, X,

$$[I + A(\alpha, ka, kd_{qj})]X = B,\ A = \{A_{m,n}^{(q,j)}\}_{m,n=-\infty,\ q,j=1}^{+\infty,\ M},\ B = \{B_m^{(q)}\}_{m=-\infty,\ q=1}^{+\infty,\ M},\ X = \{x_m^{(q)}\}_{m=-\infty,\ q=1}^{+\infty,\ M}. \quad (1)$$

Important thing is that the unknown coefficients are re-scaled in such a way that the matrix equation (1) becomes a set of linear algebraic equations of the Fredholm second kind that means,

$$\sum_{m,n=-\infty,\ q,j=1}^{+\infty,\ M} \left|A_{mn}^{(q,j)}\right|^2 < \infty,\ \sum_{m=-\infty,\ q=1}^{+\infty,\ M} \left|B_m^{(q)}\right|^2 < \infty. \quad (2)$$

This guarantees the convergence of the solutions of this equation with each block truncated to $N{\times}N$ elements, to converge to the exact solution, for larger N. The same is valid for the eigenvalues of the truncated matrix equation, in the case of the lasing eigenvalue problem. This allows all the results presented in this dissertation to have controlled accuracy, which we have limited to three or four decimal digits.

The calculation of the scattering of the H-polarized plane wave on a single silver nanowire in the visible light range (wavelengths of 300-500 nm) demonstrates a broad peak of the collective plasmon-mode resonance on the TSCS and ACS wavelength dependences, slightly shifted to the red side from the wavelength of λ = 338 nm where the real part of silver's permittivity is opposite to that of the outer space. It has a low Q factor, which is determined by the losses in silver. A widely spread opinion that the plasmon resonances are associated with nanosize metal scatterers, urged us to investigate the existance of these resonances on wires with radius greater than 100 nm. As a result, we have shown that the multipole plasmon resonances are observed on much thicker wires so far as the shaded part of wire's outer boundary does not exceed significantly the surface-plasmon wave propagation length, which grows with λ in free space, but is limited to tens and several hundred λ.

Next, the scattering of waves by linear sparse gratings of M dielectric and silver nanowires with radius from 30 nm to 70 nm is considered. At the scattering of the visible-light waves by a lossless dielectric-wire grating with period $p > 4a$, the high quality resonances are observed on the TSCS spectra at the wavelengths close to the Rayleigh anomalies (for the corresponding infinite grating), $\lambda_{RA}^{\pm m} = (\cos\varphi_0 \pm 1)p/m$, m = 1,2.., Their Q-factors increase with M. These are resonances on GM, and their characteristic features are the Fano-shape peaks in the scattering and absorption (if wires are lossy) and the presence of a standing wave along the grating, close to the function $\cos(2\pi x/p)$, formed by the propagating quasi-harmonics Floquet. For the gratings of dielectric wires, the GM resonances are observed in both polarizations, but in the case of the E-polarization, their Q-factors are smaller by a factor ε^2. Besides, in E-case the deep minima of TSCS appear at the Rayleigh anomalies, similarly to the behavior of the corresponding infinite gratings.

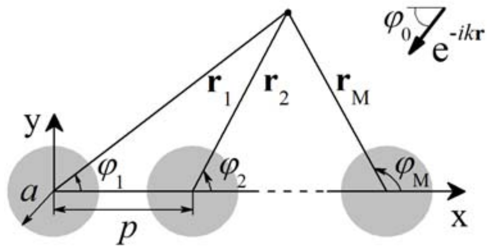

Fig. 1 Cross-section of the linear grating of circular wires under the plane wave incidence

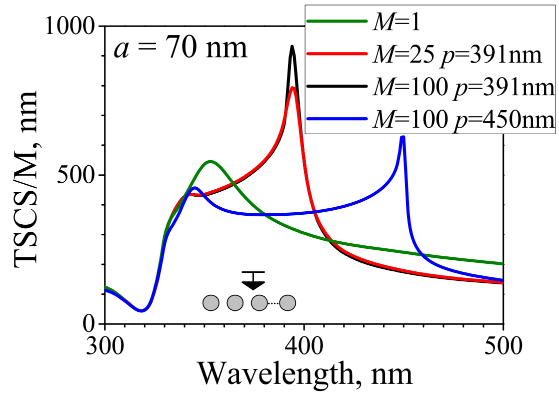

Fig. 2 TSCS as a function of the wavelength for linear gratings of silver nanowires

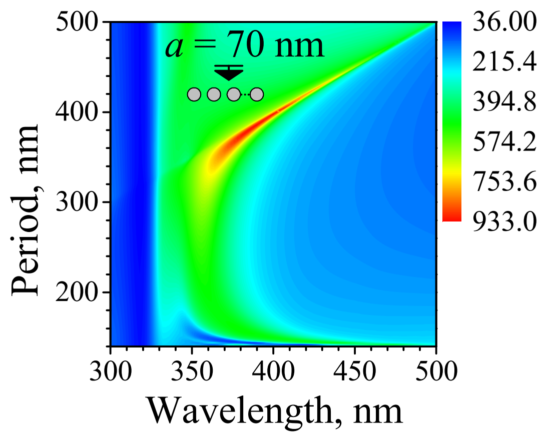

Fig. 3 Relief of TSCS as a function of the wavelength and the period for a linear grating of 100 silver nanowires

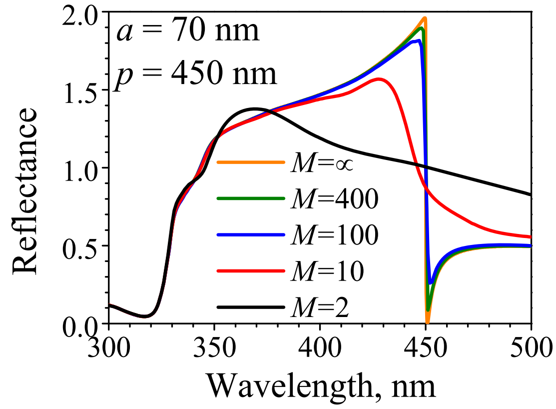

Fig. 4 Normalized reflectance as a function of the wavelength for finite and infinite gratings of silver nanowires

In the H-polarized plane wave scattering by a silver nanowire grating, both plasmon and GM resonances occur in the scattering and absorption characteristics (see Figs. 2-3). We have shown that by changing the period of the grating, the resonance peak of TSCS can obtain significantly greater sharpness in comparison with the plasmon resonance. However, at the coincidence of the wavelength of the plasmon resonance and that of the GM, i.e. the grating period (under the normal incidence), one can see the phenomenon of electromagnetically-induced transparency. At the same λ, "reflection cross-section" (see below) reaches a minimum. In the E-polarization, the plasmon and GM resonances do not occur in the scattering and absorption characteristics of such gratings, and at the wavelengths close to the Rayleigh anomalies, a suppression of the scattering and absorption occurs, similarly to the case of dielectric gratings.

We also compared the scattering by finite and infinite gratings. It was found that here one has to compare the reflection characteristic that can be called the "reflection cross-section" for a finite grating. This is the part of the TSCS assocoated with the power scattered to the upper half-space, normalized by the number of wires M and their diameter $2a$. It is to be compared, for the infinite grating, with the reflection coefficient normalized by a value of $2a/p$. In Fig. 4, presented are the wavelength dependences of such reflection coefficients for the gratings of nanowires with radius 70 nm and period 450 nm. The comparison shows that a 10-wire grating is enough to match the TSCS dependences with an accuracy of ±10% in the whole studied wavelengths range, except of the vicinity of GM resonance, where from 100 to 500 wires is needed to achieve the same effect.

Chapter 3 is devoted to the study of the scattering and absorption characteristics of the H-polarized visible-light waves by various periodically-structured configurations of finite number of silver nanowires. Considered are the configurations in the form of discrete corner, discrete cross, two-layer and three-layer finite gratings, and finite gratings with two periods. They are schematically depicted in Fig. 5. In addition, a discrete parabolic reflector (DPR) of silver nanowires is

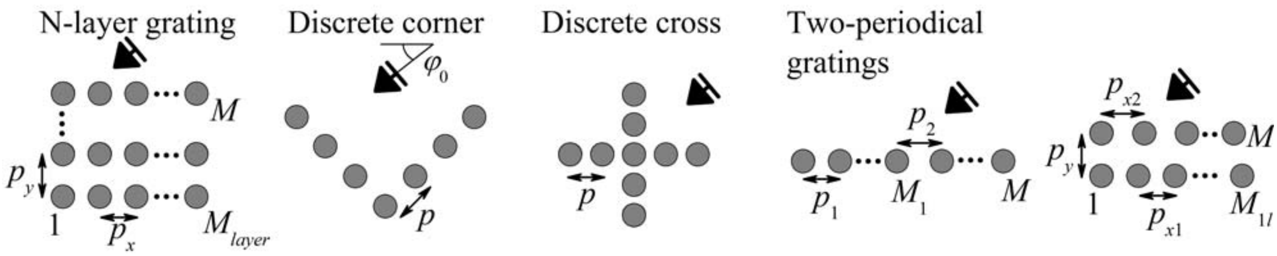

Fig. 5 Cross-sectional views of the grating configurations considered in Ch. 3

analyzed. Besides, the ability to detect a periodic structure in a clutter is studied. For this, the scattering of waves by a linear silver nanowire grating, which is in a "cloud" of pseudo-randomly located identical wires, is analyzed.

We demonstrate that in the scattering of light by all of the considered structures, the plasmon and the GM resonances occur on the frequency dependences of TSCS and ACS. In each case, the plasmon resonance always occurs near the wavelength of 338 nm and has small Q-factor, and resonances on GMs occur near the wavelengths of the Rayleigh anomalies, which depend on the angle of incidence. Their Q-factors vary and, above all, depend on the number of wires in the grating. For example, for a multi-layer grating, the addition of layers reduces the maximum values of the normalized by *M* TSCS and ACS in the GM resonance, which is caused by the shadowing of the lower layers.

Discrete right corners and discrete crosses are interesting under symmetric illumination, where a plane wave is incident under the angle 45° to each of their arms. Thus, the wavelength of the GM resonance is shifted from the value of the period of the grating (near which it is in the case of normal incidence), and the Q-factor of the GM resonance increases. In Fig. 6, presented are the reliefs of the TSCS dependences on the wavelength and the grating period. Besides, the lines corresponding to the +1-st and +2-nd Rayleigh anomalies are shown for discrete crosses of 101 silver nanowires with 30 nm radius and two cases of illumination: when a plane wave is incident along the arm of the cross ($\varphi_0 = 90^\circ$, if the cross is positioned as in Fig. 5) and along its diagonal ($\varphi_0 = 45^\circ$).

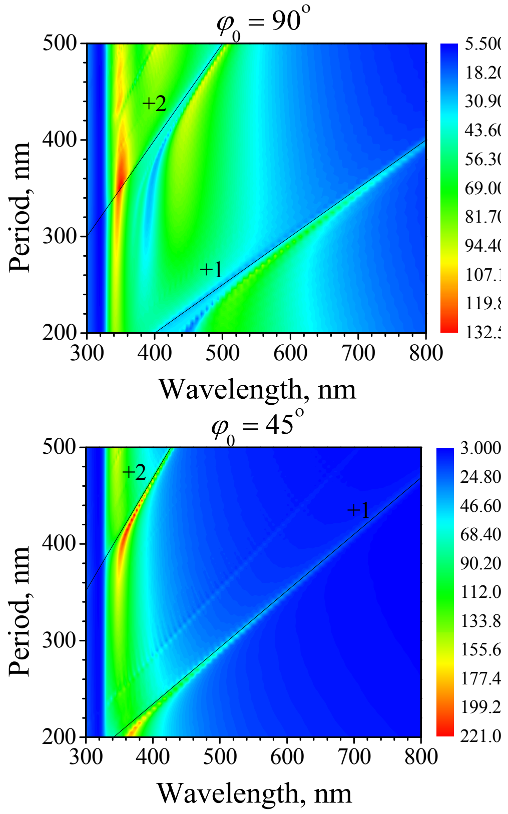

Fig. 6 Color maps of TSCS as a function of the wavelength and the period for a discrete cross of 101 silver nanowires with the radius of 30 nm

It should be noted that the amplitudes of the near field reach higher maximum values not in the plasmon resonances, but in the GM resonances. This tells that using this type of resonances is more promising than the more traditional plasmon resonances, in various sensors and optical nanoantennas, where the most important is the enhancement of the near field.

In addition, the design of a refractive index sensor based on the GM resonance is attractive because its volume sensitivity is comparable to the sensitivity of traditional sensors on plasmon resonance, but the Q-factor can be much higher provided that the number of periods exceeds 100. This makes the figure-of-merit of such a sensor (the product of sensitivity and Q-factor) greater than for traditional sensors, if only the substance being analyzed fills a layer thicker than the wavelength. Additionally, if a sensor uses a corner or a cross of nanoparticles instead of a linear grating, then it is possible to spatially separate the directions of illumination and reception of the scattered light.

High-quality resonances on GMs are also attractive for the development of nanosize thin absorbers for solar cells. This is due to the fact that such resonances can be adjusted to certain wavelengths by selecting the period values. Thus, it is possible to create bands of high absorption in those parts of the spectrum, where there are no plasmon resonances. Here, additional features may appear if using more complex configurations, which have not one, but several sub-gratings with different periods.

We consider two configurations of such gratings: two chains of nanowires with periods p_1 and p_2 located together in-line, two chains of nanowires stacked one above the other. As expected, such gratings exhibit resonances on the GMs associated with each period.

The focusing of waves using solid metal reflectors is widely used in optics and quasi-optics, and parabolic reflectors are the most common and efficient ones. As well known, the TSCS of a single stand-alone nanowire greatly increases in the plasmon resonance. Therefore, it is interesting to check how efficiently a discrete parabolic reflector (DPR) made of the resonant silver nanowires can focus the light.

Our DPR consists of *M* parallel nanowires, whose centers of cross-section are placed symmetrically on a parabolic curve at a distance *p* between adjacent ones. Here, we assume that DPR is built in such a way that the central wire coincides with the vertex of the parabola; therefore the number *M* is odd. The focus of the parabola is at the point (0; *f*), and the focal length *f* and is given by the equation $\bar{y} = a\bar{x}^2 / 4f$, where $\bar{y} = ya$, $\bar{x} = xa$. The aperture width of DPR is *D*, which is the distance between the edge wire centers. This reflector is illuminated by a plane H-wave incident normally along the *y*-axis. As known, for solid metal reflectors, the optimal value is $f / D = 0.25$. We investigate the focusing properties of DPR computing the field magnitude in the geometrical focus. Main attention is paid to the effect of the plasmon resonance of silver nanowires, as well as the effect of quasi-periodicity. Our research shows that the best focusing ability has DPR with $f / D = 0.25$ in the plasmon resonance on each wire. In Fig. 7, presented is the near field pattern in the plasmon resonance for a DPR of 51 wires with radius 70 nm and *p* = 450 nm. It has a clearly visible bright spot centered on the geometrical focus of the corresponding parabola, with peak magnitude of 5.6. As for the GM resonance, at the wavelengths close to *p* the focusing ability of DPR is low because this resonance is absent on the curved structure.

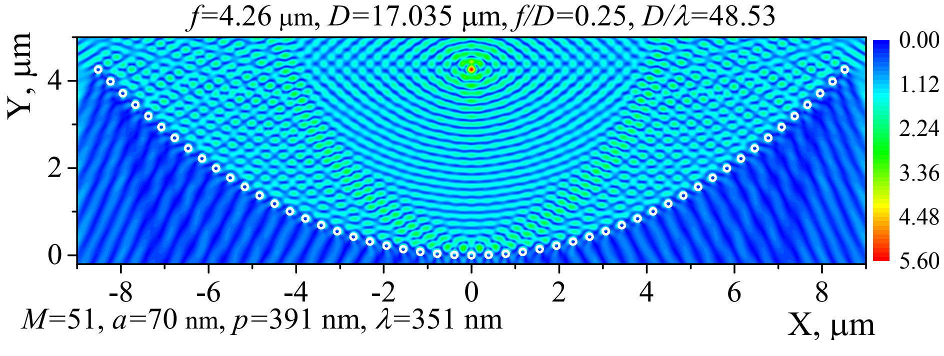

Fig. 7 Near field of DPR in the plasmon resonance

When studying the resonances on GMs, a natural question arises: how sensitive are these resonances to deviations from the periodicity, or vice versa, what is the effect produced by the periodic structuring of an arbitrary ensemble of identical scatterers. Thus, we have considered the plane H-wave scattering by a finite linear grating of M_p silver nanowires, placed in a "cloud" of M_c similar nanowires. The geometry of the cross section of such a structure is shown in Fig. 8. The cloud, in the center of which a linear grating is placed, can be defined by a virtual circle of 200 periods in diameter. Inside of it, there are pseudo-randomly located 200 wires with the minimum distance between them being 10.67a, that is, the cloud is sparse. Linear gratings, which are inserted into the cloud, have M_p = 50, 100 and 200 wires with period p = 450 nm. All wires have the same radius. a = 60 nm.

In Fig. 9, presented are the reliefs of the normalized by M TSCS as a function of the wavelength and the angle of incidence for a cloud of 200 pseudo-randomly located wires and for the same cloud with a grating of 50 wires. On the upper panel, a bright strip of plasmon resonance is visible for all angles of incidence, and no other effects are observed. It is further seen that if a grating of 50 nanowires appears in the cloud, the relief of the TSCS changes so significantly that one can see a characteristic signature of periodicity in the form of a W-shaped region of high scattering, along the lines of the Rayleigh anomalies. This feature becomes brighter for larger M_p, and if $M_p = M_c$ = 200, the strip of the plasmon resonance fades off on the background of the W-shaped GM resonance region. In addition, at the resonant wavelengths, there appear sharp lobes of the angular scattering pattern in the directions of the Floquet harmonics propagation, and additionally the intense lobes along the grating. These effects get enhanced with increase of the size of the periodic grating.

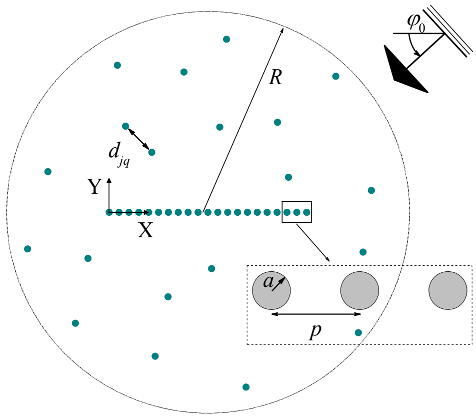

Fig. 8 Cross-section of the grating of silver nanowires inside a cloud of the same wires

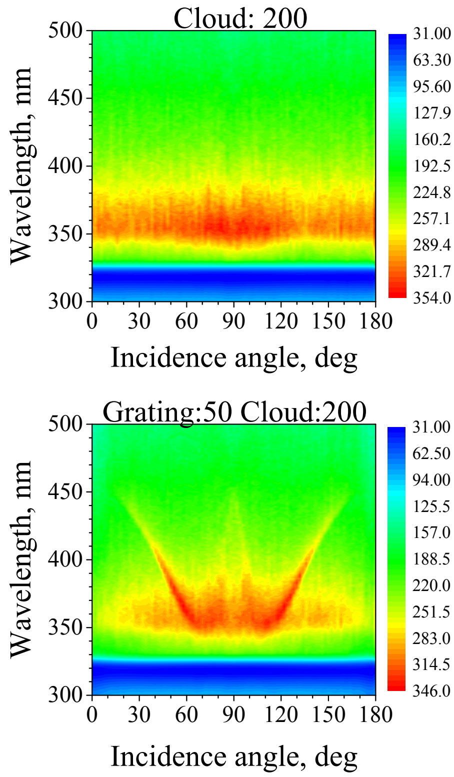

Fig. 9 Color maps of TSCS as a function of the wavelength and the incidence angle for a cloud of 200 silver nanowires and for the same cloud with the grating of 50 nanowires placed approximately in the cloud center

Chapter 4 is devoted to the electromagnetic modeling, using the lasing eigenvalue problem (LEP), of 2-D nanosize plasmonic lasers based on stand-alone silver nanowires and nanotubes, and on the periodic gratings of finite number of dielectric and core-shell silver nanowires. Within such formulation, we look for the on-threshold frequencies, self-excitation gains, and the fields of eigenmodes of nanolasers, and study their dependence on the laser geometry.

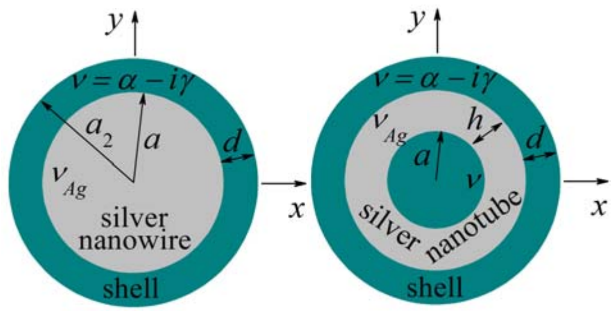

Fig. 10 Cross-sections of nanolasers based on silver nanowire and nanotube

First of all, we consider on-threshold lasers based on a single silver nanowire with an active shell and on a single silver nanotube with an active core and an active shell (Fig. 10). Since such nanolasers are interesting because of their plasmon modes, we consider only the case of the H-polarization. The radius of sub-wavelength nanolasers is $a \leq 200$ nm, and we look for the modes shining in the wavelength range from 190 nm to 700 nm. Within the LEP formulation, if the H_z field component is denoted as U, this function must satisfy 2-D Helmholtz equation with complex refractive indices ν_s (s = 1,2,3..S is the number of a domain of the nanolaser cross-section), which correspond to the problem geometry. Namely, in the active regions, $\nu = \alpha - i\gamma$, where α is known refractive index and γ is unknown gain index, i.e. self-excitation threshold. It is assumed that the gain is uniformly distributed throughout the active region and does not depend on the wavelength. On the boundaries of the partial domains, the conditions of the continuity of the tangential field components are imposed, and also Sommerfeld radiation condition at infinity and condition of the local power finiteness must be satisfied.

The separation of variables leads to the splitting of all modes into independent orthogonal families by the azimuthal index m, as well as symmetry and anti-symmetry according to the chosen direction $\varphi = 0$. In solving the LEP, the separation of variables allows us to proceed to independent transcendental characteristic equations $\det \hat{T}(m, \lambda, \gamma) = 0$ for the modes of each index m = 0,1,2… and investigate them separately. Finite-dimensional matrix operator $\hat{T}$ of the characteristic equation contains Bessel and Hankel functions of index m with arguments, which contain refractive indices of all materials of nanolaser.

For numerical search of the LEP eigenvalues (λ, γ), which are the roots of the characteristic equation, we use an iterative Newton-type algorithm, which needs initial-guess values of the sought quantities. Due to the strong dispersion of permittivity of silver, as well as the fact that such modes are relatively unexplored, we take the initial-guess values near the minima on the reliefs of the functions $|\det \hat{T}(m, \lambda, \gamma)|$. Bulk silver permittivity $\varepsilon_{Ag}(\lambda)$, as in the previous chapters, is taken from experimental data of Johnson and Christy and interpolated by splines.

The analysis of the self-excitation thresholds and the wavelengths of the eigenmodes of the nanolaser based on a silver nanowire with active shell shows the presence of several plasmon modes with the same azimuthal index, as well as the shell modes, if the thickness of the shell is sufficiently large (> 80 nm). The most important mode of such lasers is the dipole plasmon mode P_1 , whose wavelength is in the visible spectrum, λ = 400-600 nm, if α = 2.25. It has rather low self-excitation threshold, γ = 0.2 to 0.5. The secondary plasmon modes, as well as the shell modes, have their wavelengths in the region of high losses in silver and, due to that fact, have high thresholds. The optimum radius of a silver nanowire for such a nanolaser is 40-60 nm, and the thickness of the shell is 20-100 nm.

We have also carried out a comparative analysis of the modes of silver nanowire laser using several analytical methods for the description of $\varepsilon_{Ag}(\lambda)$ (the classical Drude formula and its modifications) and the data of Johnson and Christy. We have found that the use of the classical Drude formula leads to a shift of the plasmon mode wavelength to the violet part of the spectrum and no secondary plasmon modes are present. The use of the modified Drude formula gives a good coincidence with the experimental data, except the part of the range where Im ε_{Ag} possesses negative values, which have no physical sense.

The configuration of nanolaser based on a silver nanotube with active core and shell is more attractive, because in addition to the outer boundary, there is also the inner one between the metal and active core, which also supports its surface plasmon modes. The analysis of the modes of such nanolasers shows the hybridization of the plasmon modes. This occurs due to the presence of two boundaries, provided that the nanotube is thinner than the skin-depth in the visible range (10-20 nm). As a result, the modes P_m^+ and P_m^- with field maxima at both boundaries, inner and outer, appear. The most attractive working mode of such nanolasers is the "difference" dipole mode P_1^-, which emits in the yellow or green parts of spectrum and has a low self-excitation threshold, γ = 0.1. The optimum configuration is found to be a silver nanotube laser with the core of 30-50 nm radius and 10-nm thickness silver nanotube coated with a 10-nm thick shell. An increase of the tube thickness leads to the destruction of the hybridization of the plasmon modes. In Fig. 11, presented are the trajectories of eigenvalues of lasing modes on a plane (λ, γ) for a nanotube laser if tube thickness changes.

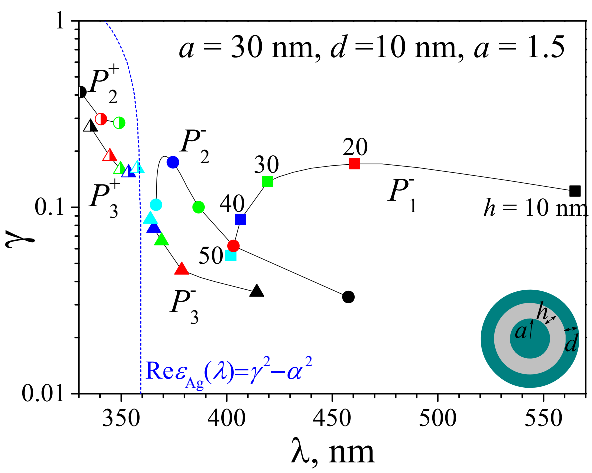

Fig. 11 Trajectories of the eigenvalues of silver nanotube laser modes under a variation of its thickness (in nm)

The observation of high quality GM resonances in the light scattering by finite gratings of dielectric and silver nanowires, investigated in Chapters 2 and 3, suggests the presence of modes with low self-excitation thresholds in corresponding LEP eigenvalue problems.

Therefore, we have considered LEP for the lasers based on nanowire gratings. here, we consider a grating of M quantum (i.e. uniform active-dielectric) nanowires with complex refractive index $\nu = \alpha - i\gamma$, and a grating from M silver nanowires with refractive index $\nu_{Ag}(\lambda)$, covered with the active shells (with $\nu = \alpha - i\gamma$).

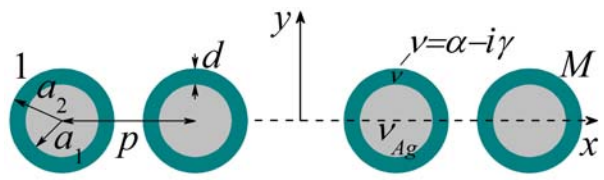

Fig. 12 Cross-section of the grating of M silver nanowires with active shells

The latter one is schematically presented in Fig. 12. The field expansion in the azimuth series in each of the partial regions, as well as the algorithm for obtaining a block-matrix equation for the unknown coefficients of field expansion, for the grating of quantum wires, are the same as in the wave-scattering problem.

For a grating of silver wires covered with active shell, two of unknown coefficients of the field function in the shell are added for each index m. As a result, we obtain a homogeneous Fredholm second-kind block-type matrix equation. This means that its determinant exists as a function of the parameters of LEP, i.e. the values (λ, γ), which are the wavelength and the threshold gain of the lasing mode. Thus, LEP is reduced to finding the roots of an infinite determinant equation,

$$\det\left\{\delta_{mn} + A_{m,n}^{(q,j)}(\lambda,\gamma)\right\}_{\substack{m,n=-\infty \\ q,j=1}}^{\infty,M} = 0. \tag{3}$$

Here, the Fredholm nature of the matrix operator guarantees that the zeros of the truncated determinant converge to the exact ones if the truncation order gets larger. The roots of finite-order analog of (3) can be found by various numerical methods. We use the secant method.

We analyze the gratings made of even number of nanowires and place the center of the global coordinate system in the middle point of the grating, which has two lines of symmetry: the coordinate axes x and y. The account of the symmetry reduces the matrix size that leads to more efficient numerical solution. It is also important, how close the initial-guess value is to the sought solution. For the grating modes, we take the initial-guess values of λ as the wavelengths of the resonance peaks of TSCS spectra in the corresponding scattering problem with the plane wave normal incidence. Initial-guess value of γ can be arbitrary small number. Usually, the

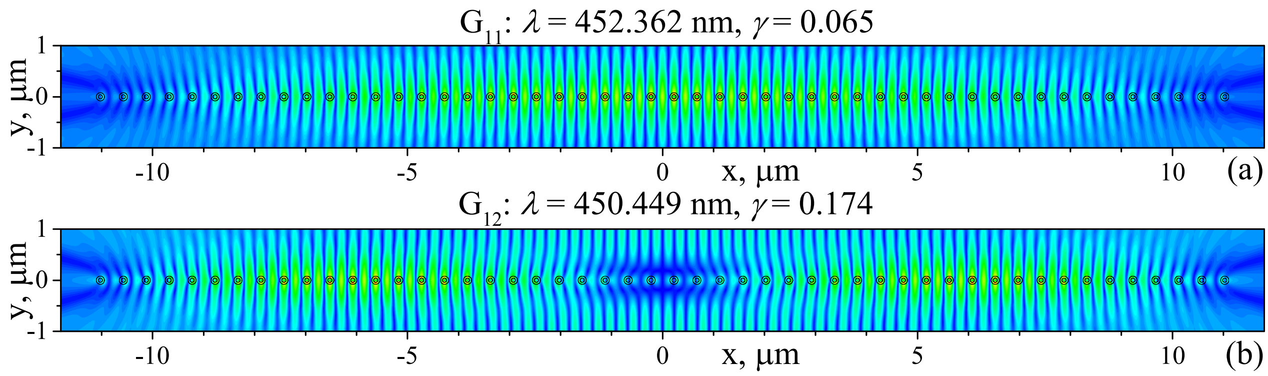

Fig. 13 Near fields of the grating modes G_{11} and G_{12} of the grating of 50 silver nanowires with the core radius a = 40 nm and active shells with α = 1.414 and the thickness d = 40 nm, collected in the grating with period p = 450 nm

coincidence of the resonant wavelength with the emission wavelength of the GM is one to two decimal digits.

Thus, we have investigated the grating modes. However, in general, in the visible-light range the gratings of nanowires have large number of eigenmodes that grows with M. This can be verified by plotting the (λ,γ) relief of the absolute value of determinant (3). Still, the grating modes are different from the other types, because of much lower self-excitation thresholds, $\gamma = 10^{-2}$ to 10^{-3}. The grating modes whose wavelengths coincide with the wavelengths of the corresponding GM resonances have the lowest self-excitation thresholds, and their fields, in which the most of the wires shine, are symmetric relatively to both coordinate axes. We call these modes the principal grating modes. Still on the gratings with large M, besides the principal GM, there are others, which can be characterized by introducing the second index n, which indicates how many "bright" parts of the grating are present in the near field of such a mode (for the principal GM, n = 1). In Fig. 13, presented are the fields of the principal GM (i.e. G_{11}) and the mode with n = 2 (i.e. G_{12}) for the grating of 50 silver nanowires of radius 40 nm coated with 40-nm active shells with α = 1.414, and the grating period is 450 nm. Further, Fig. 14 shows the trajectories of these modes (their LEP eigenvalues) under the variation of the wires number M. One can see that with increasing of the number of nanowires in the grating, the self-excitation threshold gain values of the grating modes drop down significantly, and the fastest decrease is around the maximum studied value of M, i.e. 200. We have also investigated the grating modes dynamics under the change of the other parameters, such as the radius of the wire, the shell thickness, and its refractive index.

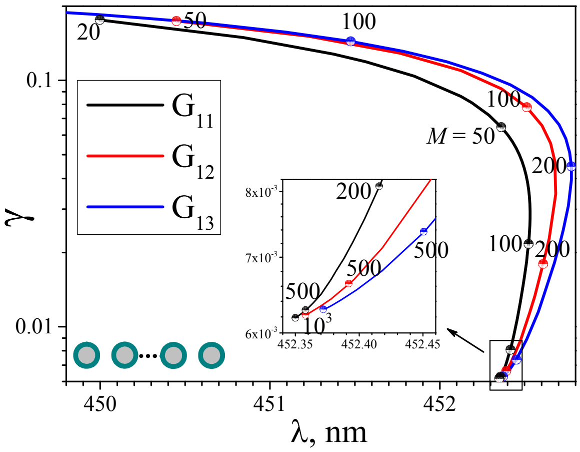

Fig. 14 Trajectories of the LEP eigenvalues of modes G_{11}, G_{12} and G_{13} on the plane (λ,γ) for the gratings of Fig. 13 if the wires number M varies

Conclusions

In the thesis, a mathematically grounded numerical algorithm with guaranteed convergence is developed for the analysis of the scattering of electromagnetic waves by finite gratings of material wires of the circular cross-section. This problem is reduced to the solution of the infinite Fredholm second kind block-type matrix equation. Truncation of each block to a finite number allows obtaining a solution with given accuracy if that number is taken greater. By following this approach, the wave-scattering and absorption characteristics, as well as the near-field patterns of linear gratings, discrete corners, discrete crosses, discrete parabolic reflectors, multilayer gratings, and gratings with several periods, made of finite number of silver and dielectric nanowires are investigated. In addition, using determinant equations based on the above-mentioned Fredholm second-kind matrix equations, the eigenmodes of plasmon nanolasers based on silver nanowires and nanotubes, as well as on the finite gratings of dielectric and silver nanowires are analyzed.

The main scientific and practical results are as follows:

- the resonances on high-quality grating modes in the scattering and absorption of electromagnetic waves by finite gratings of dielectric nanowires have been numerically investigated with guaranteed accuracy; their resonant fields have been investigated, it has been demonstrated that the sharpness of such resonances depends on the number of wires in the grating;
- in the visible-light range, two types of resonances in the scattering and absorption of the H-polarized plane electromagnetic waves on finite metal nanowire gratings have been demonstrated: on the plasmon and the grating modes;
- mutual influence of resonances on the low-quality plasmon modes and the high-quality grating modes has been investigated; it has been shown that if the real parts of their eigen-frequencies coincide, the phenomenon of electromagnetically-induced transparency is observed;
- the possibility of the focusing of the visible-light waves with quasiperiodic discrete parabolic reflectors of metal nanowires has been investigated; under the excitation of plasmon resonance on each of the wires, the focusing is most efficient; the effect of the grating-mode resonances for such reflectors is absent;
- the reflection coefficients of finite and infinite gratings of silver nanowires have been compared; it has been shown that near the frequencies of the grating-mode resonances a large finite grating (with over 100 wires) is needed to produce the reflection coefficient close to that of the infinite grating; this is much larger than off that range, where it is enough to have a finite grating of 10 wires;
- a W-shaped "optical signature of periodicity" has been demonstrated, which appears on the reliefs of the total scattering cross-section as a function of the wavelength and the angle of incidence in the form of regions of its high values; these regions stretch along the lines of Rayleigh anomalies of the corresponding infinite gratings, with a slight red shift; they are well visible even for a grating of 50 silver nanowires in the "cloud" of large number of arbitrarily located similar wires;
- within the classical electromagnetics, the frequencies, self-excitation thresholds gains, and fields of the eigenmodes of nanolasers based on silver nanowires and nanotubes with active shell and core (in the case of a nanotube) have been found; the principal and several secondary plasmon modes have been found, in each azimuth family; the effect of various parameters on the frequencies and self-excitation thresholds of their eigenmodes have been investigated;
- the grating modes of finite gratings of dielectric and silver nanowires have been found and classified; it has been demonstrated that their self-excitation threshold gains are much lower than of the other modes, and their wavelengths well agree with the wavelengths of the corresponding resonances in the scattering problems.

List of main publications related to the thesis

1. D. M. Natarov, V. O. Byelobrov, R. Sauleau, T. M. Benson, A. I. Nosich, Periodicity-induced effects in the scattering and absorption of light by infinite and finite gratings of circular silver nanowires, *Optics Express*, vol. 19, no 22, pp. 22176-22190, 2011.
2. D. M. Natarov, R. Sauleau, A. I. Nosich. Periodicity-enhanced plasmon resonances in the scattering of light by sparse finite grids of circular silver nanowires, *IEEE Photonics Technology Letters*, vol. 24, no 1, pp. 43-45, 2012.
3. D. M. Natarov, R. Sauleau, A. I. Nosich, Resonance scattering and absorption of light by finite two-period gratings of circular silver nanowires, *Int. J. Semiconductor Physics, Quantum Electronics, and Optoelectronics* (ISP NASU Press), vol. 15, no 3, pp. 204-208, 2012.
4. D. M. Natarov, R. Sauleau, M. Marciniak, A. I. Nosich, Effect of periodicity in the resonant scattering of light by finite sparse configurations of many silver nanowires, *Plasmonics*, vol. 9, no 2, pp. 389-407, 2014.
5. D. M. Natarov, Modes of a core-shell silver wire plasmonic nanolaser beyond the Drude formula, *IOP J. of Optics*, vol. 16, no 6, pp. 075002/6, 2014.
6. D. M. Natarov, M. Marciniak, R. Sauleau, A. I. Nosich, Seeing the order in a mess: optical signature of periodicity in a cloud of plasmonic nanowires, *Optics Express*, vol. 22, no 23, pp. 28190–28198, 2014.
7. E. A. Velichko, D. M. Natarov, Localized versus delocalized surface plasmons: dual nature of optical resonances on a silver circular wire and a silver tube of large diameter, *IOP J. of Optics*, vol. 20, no 7, art. no 075002/9, 2018.
8. D. M. Natarov, O. V. Shapoval, M. Marciniak, A. I. Nosich, Rayleigh anomalies in the E-polarized scattering by finite flat gratings of silver nanostrips or nanowires, *Proc. Int. Conf. Mathematical Methods in Electromagnetic Theory (MMET-2012)*, Kharkiv, 2012, pp. 44-47.
9. D. M. Natarov, M. Marciniak, R. Sauleau, Modeling of discrete parabolic reflector made of sub-wavelength plasmonic wires, *Proc. Int. Symp. Physics and Engineering of Microwaves, MM, and Sub-MM Waves (MSMW-2013)*, Kharkiv, 2013, pp. 455-457.
10. D. M. Natarov, Electromagnetic analysis of a silver nanowire laser with a concentric active region, *Proc. URSI General Assembly and Scientific Symp. (URSI-GASS-2014),* Beijing, 2014, art. no BP1.37.
11. D. M. Natarov, Grating resonances in the scattering of light by periodically structured dielectric nanowires, *Proc. Int. Conf. Mathematical Methods in Electromagnetic Theory (MMET-2016)*, Lviv, 2016, pp. 236-238.
12. D. M. Natarov, Lasing thresholds of plasmonic modes of a silver tube nanolaser with active shell and core, *Proc. IEEE Ukraine Conf. Electrical Computer Eng. (UKRCON-2017)*, Kiev, 2017, pp. 748-751.
13. D. M. Natarov, Analysis of eigenmodes of laser based on finite quantum nanowire grating, *Proc. Int. Workshop on Direct and Inverse Problems of Electromagnetic and Acoustic Wave Theory (DIPED-2018)*, Tbilisi, 2018, pp. 76-79.