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ELECTROMAGNETIC FIELDS AND SELF- EXCITATION THRESHOLDS OF PERIODIC RESONATORS MADE OF DIELECTRIC, METALLIC AND QUANTUM WIRES IN LAYERED MEDIUM

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GENERAL DESCRIPTION

This work deals with analysis of natural electromagnetic fields (modes), and their frequencies and self-excitation thresholds for periodic open resonators made of dielectric, metallic and quantum wires located, in general, in a flat-layered dielectric medium. As auxiliary problems, we also study two-dimensional problems of the time-harmonic plane-wave scattering by infinite gratings of circular dielectric and metallic wires. Under the term “quantum wires” we understand, as usual in nanotechnology, the wires of the material with gain. Such materials can be semiconductors, dye-doped polymers, and crystals doped with ions of rare-earth elements. They all can enhance the spontaneous emission of light under pumping thanks to creation of inverse population of quantum levels. Our analysis is based on the boundary-value problems for the Maxwell equations which are cast to the matrix equations of the Fredholm second kind.

Timeliness of the topic. Modern systems and devices of communication and information processing with the aid of electromagnetic waves are quickly mastering the short-wave ranges from the terahertz to the ultra-violet. Therefore the sources of such waves are actively developed now. Here, the vacuum electronics devices are absent or provide very small powers and therefore the most promising sources are lasers based on the crystalline, polymer and semiconductor microcavities (with the size from units to a few hundred microns) and arrays of nanocavities (with the size from a few dozen to a few hundred of nanometers). Active regions in these lasers are created thanks to quantum properties of semiconductors or by doping the polymer matrix with dyes or the crystalline material with ions of rare-earth elements. The desired shaping of the resonators is achieved by the use of nanotechnologies, such as molecular-beam epitaxy and dry and wet etching. The pumping is arranged either optically or via injection of carriers from the electrodes.

From the above mentioned it becomes clear that the fabrication of microlasers based on stand-alone resonators or arrays of nanoresonators requires access to extremely expensive technologies. Still further problems are associated with measurements of their characteristics, especially in the terahertz range. Only a relatively moderate number of laboratories in the world are engaged in the development and experimental research into such lasers. In Ukraine, such technologies are absent. Because of these circumstances, a preceding modeling of the mentioned lasers and an optimization of their geometries already at the design stage, i.e. before manufacturing, obtain crucial importance.

It is necessary to emphasize that the development of efficient micro and nanolasers calls for accurate account of their geometries and material parameters as their dimensions are comparable to the wavelength of emission. Further, one of the fundamental properties of lasers is their ability to emit light on discrete wavelengths. This is directly connected to the conception of *natural modes* as discrete forms of electromagnetic field in the resonators. Therefore any laser can be viewed as an open resonator equipped with an active region able to generate the electromagnetic waves under the pump.

Until recently, the methods of modeling of laser resonators dealt only with the search for complex frequencies of natural modes of *passive resonators* without any account of the presence of active region. One the most widespread was the Geometrical Optics (GO) or the billiard theory. However this method cannot provide a reasonable accuracy of modeling of the resonators sized in dozens of wavelengths, is not able to estimate the losses for radiation and hence the Q-factors of modes, and completely fails in the description of fields in periodic resonators.

The other popular instrument, numerical method of finite differences in time domain (FDTD), although useful in other areas, is not applicable to the direct study of natural modes. Instead, it requires placing a pulse source into a resonator, computing time-dependent field at some point and finding the mode Q-factors with the aid of numerical Fourier transformation. Each of the mentioned operations brings considerable and uncontrolled errors that lower FDTD's accuracy.

The mentioned circumstances point out to the necessity of modeling the microlasers, including those shaped as arrays of nanoscale elements, by using the methods of theory of boundary-value problems for the time-harmonic Maxwell equations with exact boundary conditions and radiation condition at infinity.

Still any analysis of the natural modes of *passive open resonators* is considerably devaluated by the absence, in such model, of any opportunity to reproduce one other fundamental property of a laser: the existence of the threshold of self-excitation (i.e. the threshold value of pump power). The earlier proposed ways to introduce the thresholds were based on quantum-mechanical nonlinear models despite a physically obvious observation that "at the threshold" the amplitude of electromagnetic field is negligibly small and thus the analysis of self-excitation thresholds must not require account of nonlinear effects.

The mentioned drawback was overcome when in the 2000s, in the works of A. I. Nosich and E. I. Smotrova, it was first proposed to study lasers as *open resonators with active regions*, filled with a gain material. In that case one can formulate a Lasing Eigenvalue Problem (LEP), in which every eigenvalue is a pair of real numbers: the emission frequency and the associated threshold value of gain in the active-region material. Using this approach, the modes of two-dimensional microlasers were analyzed; this included cyclic photonic molecules of active circular resonators and the active stand-alone resonators of complicated shapes. Still previously the LEP approach was not applied to the analysis of the mode frequencies and thresholds of lasers based on periodic structures. Meanwhile, quick development of nanotechnology and nanophotonics has led, in the past 10-12 years, to very active research into the effects of anomalous (i.e. resonant) transmission of optical, infrared and terahertz waves through periodically perforated layers and their anomalous reflection from rare gratings of nanoparticles. It has become clear that such periodic structures are, in fact, specific open resonators that can support whole new class of natural modes with very high Q-factors – the grating or lattice modes.

At first, their area of application was found in the design o resonant bio-chemical sensors of the host medium refractive index. However by today the focus of research has shifted to the research and development of novel lasers based on the gratings made of metallic, dielectric and quantum particles placed on a flat-layered substrate. Their working modes are the mentioned above grating modes and such sources are called “plasmonic” or “hybrid distributed feedback lasers.” The number of periods in such devices is usually large and counted in hundreds to thousands that justifies their electromagnetic modeling as infinite gratings.

In view of above mentioned considerations, the topic of research is modern and timely.

Relation to R&D programs and projects. The research related to the thesis was performed in the Laboratory of Micro and Nano Optics of IRE NASU in the framework of the following projects:

1. Research project of NASU “Development and application of new methods of computational radio-physics and theoretical and experimental research into transformation of electromagnetic fields of gigahertz and terahertz ranges in objects and media of man-made and natural origin” (code “Buksir-3,” state registration number 0106U011975, 2007-2010).
2. Research project of NASU “Development of optical and quasi-optical methods for establishing the regularities and peculiarities of the interaction of terahertz waves with physical and biological objects (code “Oreol,” state registration number 0111U001079, 2012-2016).
3. Competitive Target Program of NASU “Nanostructured systems, nano-materials and nanotechnologies”: project “Micro and nanoscale electromagnetic modeling of optical fields in resonators with active regions of quantum layers, wires and dots” (code “Porig,” state registration number 2007–2009).
4. National Target Program “Nanotechnologies and nanomaterials,” project “Fundamental mathematical and numerical research into optical electromagnetic fields of stand-alone and coupled microcavity lasers with nanoscale active layers, wires and dots” (code “Svitlo,” state registration number 0110U004737, 2010 -2014).
5. Competitive research project of the Ministry of Education and Science, Ukraine “Innovative numerical modeling of quasi-optical focusing systems” (code “Fokus,” state registration number 0109U005351, 2009-2010).
6. Program of exchange of NASU with the Royal Society, UK, joint projects with the University of Nottingham “Modelling of micro and nano-scale resonators and lenses for dense photonic circuits” (2006-2007) and “Advanced modelling of single and periodic active dielectric resonators for microlasers” (2007-2009).
7. Program of exchange of NASU with the Turkish State Committee for Science and Technology, jointly project with the Bilkent University, Ankara, “Innovative electromagnetic modeling of multielement quasioptical focusing systems for sub-mm and terahertz ranges” (#106E209, 2007-2009).
8. Program of exchange of NASU with AS of the Czech Republic, joint project with the Institute of Photonics and Electronics of ASCR, Prague “Elec-

tromagnetic and numerical modelling of active and nonlinear microcavities for semiconductor lasers and all-optical switches" (2008-2009).

The work was also connected to the following doctoral student fellowships of international societies and foundations:

- «Electromagnetic analysis of natural modes in distrubuted-Bragg-reflector resonators containing active regions», IEEE Antennas and Propagation Society Doctoral Research Award (2007);

- «Lasing modes in a dielectric slab microresonator with a periodic active region», International Visegrad Fund jointly with IPE ASCR, Prague, (2009-2010);

- «Modeling of frequency-selective polarizing reflectors made of sub-wavelength wire grids for millimeter-wave and THz applications» (2011-2012) and «Modeling of biosensors based on the periodic grating of silver nanoscale cylinders embedded in a dielectric layer» (2014), European Science Foundation jointly with the University of Nottingham, UK.

Aims and specific problems. The aim of research of the thesis is the analysis of natural fields (modes) of three types of open dielectric resonators with active regions. The first is flat-layered dielectric resonators. The second is infinite gratings made of dielectric, metallic and quantum circular nanowires located in the free space. And the third is various combinations of the first two types, i.e. flat-layered dielectric configurations with embedded gratings of silver and quantum wires. For each model, we study both a scattering problem and a lasing eigenvalue problem.

In the first case, we consider reflection, transmission and absorption of plane waves of two polarizations, incident normally on the grating resonators. In the second case, a dielectric structure (with silver nanowires or without them) is considered as an open resonator with active region. Then we look for the natural electromagnetic fields (modes) and corresponding to them frequencies of emission and thresholds of self-excitation. Such analysis enables us to show the ways for the lowering of the thresholds. To achieve these aims, we consider the following specific problems:

• Creation of efficient mathematical model for the computation of wave scattering and absorption by an infinite grating of circular wires,

• Systematic computations of the coefficients of reflection, transmission and absorption of plane waves and search for the resonance phenomena cause by the existence of natural modes,

• Creation of mathematical model, which provides adequate description of natural electromagnetic fields (modes) of periodic open resonators made of nanowires,

• Development of numerical algorithms for the computation of natural fields, frequencies and thresholds of self-excitation for the modes of infinite gratings made of quantum nanowires,

• Systematic computation of natural electromagnetic fields (modes), their frequencies and thresholds of self-excitation for periodic open resonators made of dielectric, metallic and quantum nanowires.

The object of research is the phenomena of the electromagnetic wave emission and scattering by periodic open resonators shaped as infinite gratings made of circular dielectric, metallic and quantum wires located, in general, in a flat-layered medium.

The subject of research is the natural electromagnetic fields (modes), their frequency spectra and self-excitation thresholds, and also the resonance fields in the scattering of waves by the above mentioned gratings.

Methods of research. The work uses the methods of the theory of electromagnetics boundary-value problems for periodic structures with exact boundary conditions, condition of periodicity, and radiation condition. These problems are cast to the infinite matrix equations of the Fredholm second kind. Eigenvalues are the frequencies and the thresholds of self-excitation and they are found numerically as the roots of the corresponding determinantal equations. Material properties of metals in the optical range of wavelengths are taken from the experimental data.

Scientific novelty of obtained results follows from the following achievements:

- The nature of so-called grating or lattice modes of the periodic open resonators made of thin dielectric or metal wires was established
- It was discovered that the grating modes of infinite grating of quantum nanowires can have ultra-low thresholds of self-excitation
- It was demonstrated that the self-excitation thresholds of the grating modes can be further lowered by making larger the distance between the quantum wires, by making smaller their refractive index, and placing the quantum wires between two distributed Bragg reflectors
- It was demonstrated that, in the scattering and absorption of waves in the optical range of wavelengths by a grating of metallic nanowires and a binary grating of dielectric and metal nanowires, the resonances on the surface-plasmon modes and on the grating modes exist together
- It was discovered that in a binary grating of quantum and metal nanowires the self-excitation thresholds of the grating modes can be lower than of the surface-plasmon modes
- Based on the Maxwell equations, the Poynting theorem was established for the modes of periodic open resonator of nanowires that links the threshold gain with the mode field characteristics
- The asymptotic expressions for the frequencies and thresholds of self-excitation of the grating modes of infinite grating made of circular quantum wires were derived, valid if the wire radius or refractive-index contrast tend to zero

Practical importance of obtained results. The developed in the thesis approach and corresponding numerical algorithms can be used in electromagnetic analysis and optimization of working modes of laser microresonators with periodically structured active regions or with metallic nanowires gratings. The established characteristics of such modes deepen considerably our understanding of behavior of their thresholds of self-excitation in the presence of periodicity. They also show the possible ways for the lowering of the thresholds.

Personal contribution of the candidate. All main results presented in the thesis were obtained by the author. His contribution in the research papers [1-6,9-11] is in the derivation of basic equations, development of numerical algorithms, systematic computing of mode frequencies and thresholds, and also interpretation of the results related to infinite gratings of nanowires; in review papers [7,8], it is in the computations required to illustrate the resonances on the grating and plasmon modes in wave scattering by the gratings of silver nanowires.

Dissemination of results. The thesis results have been presented and discussed at the following scientific seminars: IRE NASU (head Prof. P. M. Melezhik), Kharkiv University of Air Force (head Prof. O. I. Sukharevsky), Erciyes University, Kayseri (head Prof. M. Turkmen), and George Green Institute for Electromagnetics Research of the University of Nottingham (head Prof. T. M. Benson). They were also presented at the following international conferences and symposia:

• IEEE Mediterranean Microwave Symposium, Budapest (2007)
• Optical Waveguide Theory and Numerical Modeling, Copenhagen (2007), Eindhoven (2008), Barcelona (2012), London (2015)
• Theoretical and Computational Nanophotonics, Bad Hoffen (2008)
• SPIE Photonics Prague, Prague (2008)
• Transparent Optical Networks, Rome (2007), Athens (2008), Ponta-Delgada (2009), Munich (2010), Stockholm (2011), Coventry (2012), Cartagena (2013)
• Asia-Pacific Microwave Conference, Yokohama (2010)
• European Microwave Conference, Manchester (2011)
• European Conference on Microwave Integrated Circuits, Amsterdam (2012)
• IEEE Conference on Mathematical Methods in Electromagnetic Theory, Kharkiv (2012), Dnipro (2014), Lviv (2016)
• IEEE Conference on Electronics and Nanotechnology, Kyiv (2013, 2016)
• Microwaves, Radar and Wireless Communications, Gdansk (2014)
• IEEE Conference on Advanced Optoelectronics and Lasers, Alushta (2008), Sevastopol (2010), Sudak (2013), Odesa (2016)
• IEEE Conference UKRCON, Kyiv (2017)

Publications. The **r**esults obtained in the course of thesis research were published in 48 papers that includes 7 journal papers [1-7], one chapter in collective book [8] and 40 papers in the proceedings of international conferences, 3 of which are included into the given below list of main publications.

Structure and volume of thesis. The thesis includes introduction, 5 chapters, conclusions, and the list of references. The total volume counts 193 pages, from which 10 pages are for the list of references (143 titles).

BRIEF DESCRIPTION OF THE WORK

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

Chapter 1 presents an overview of the literature around the topic of dissertation. General information is given on various approaches and on the earlier results of studying the lasers as open resonators with active regions. Research into the modes of 1-D flat-layered dielectric resonators and associated numerical methods is reviewed that is followed by the review of methods and publications on the scattering by plane waves by infinite gratings of circular wires. Explained are the drawbacks and limitations imposed by the passive-resonator model. Then the Lasing Eigenvalue Problem is formulated for a generic open resonator equipped with an active region. For such a resonator, the Optical Theorem is presented to explain the link between the threshold gain value and the mode field overlap coefficient with active region.

In Chapter 2, we study the frequencies and thresholds of modes of a flat-layered dielectric resonator, which contains a layer of the gain material.

First of all, it is necessary to note that in today's photonics the flat-layered semiconductor micro-cavities with embedded into them active layers ("quantum wells" or layers of random quantum dots) occupy a very important place. In particular, such structures are found in the widely known vertical cavity surface emitting lasers (VCSELs).

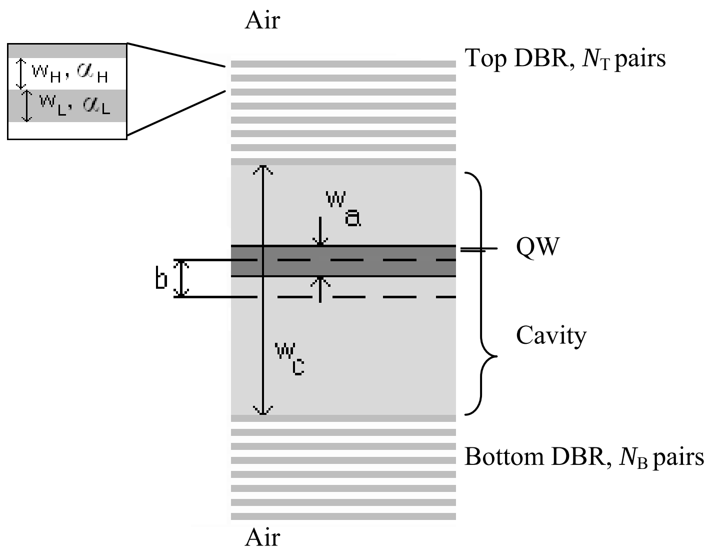
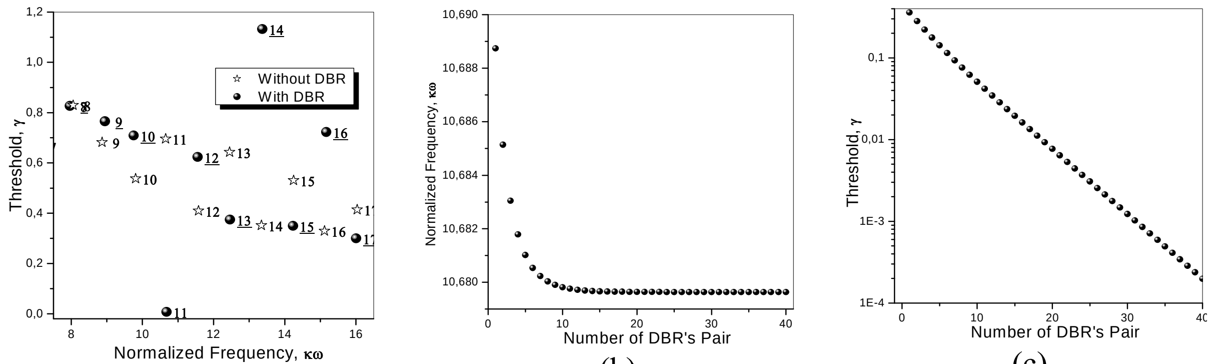


Fig. 1. Cross-sectional view of a flat-layered dielectric open resonator with an active layer

In the simplified 1-D model, a VCSEL is made of a flat resonator containing an active layer and two mirrors made of distributed Bragg reflectors (DBR), see Fig. 1. For understanding the emission modes of VCSEL, one has to study at first the modes of the flat resonator that makes its core. Such a simple resonator is called "Fabry-Perot etalon."

If the DBR reflectors are absent and the active layer is placed exactly in the resonator center, then $b=0$ and the geometry is symmetric. Then the LEP can be reduced to characteristic equation, $e^{-i2\kappa(\alpha_c - i\gamma)(w_a/w_c)} = R_1 R_2$, where $R_1 = R_2$ are the reflection coefficients of the lower and upper dielectric-air interfaces. The asymptotic expressions for the roots of this equation depend on the relative width of the active region, w_a / w_c, and the index of refraction, $\alpha_c >> 1$, as follows:



(a) (b) (c)

Fig. 2. Effect of DBRs on the self-excitation thresholds of a GaAs resonator with an active layer of the width w_a=0.1w_c in its center: w_H =79.63 nm, w_L =69.48 nm (a). Dependence of the normalized frequency (b) and the threshold gain (c) of the mode E_{11} on the number of pairs of layers in DBRs.

$$\kappa_n = \pi(n+1)/\alpha_c, \qquad \gamma_n = [\kappa_n(w_a / w_c)]^{-1} \ln[(\alpha_c + 1)/(\alpha_c - 1)], \qquad (1)$$

where $\kappa = kw_c$ is the normalized frequency, γ is the threshold value of gain needed for the mode self-excitation. For the numerical analysis of similar LEP for the full model of VCSEL, we use the transfer-matrix method and modified characteristic equation where the coefficients R_1 and R_2 are replaced with DBR's reflection coefficients.

In Fig. 2, we show the results of computation of LEP eigenvalues for the full model of Fig. 1. Here, semiconductor layer of the thickness w_c is made of GaAs with refractive index $\alpha_H = 3.53$ and contains, in its center, the active layer of the thickness $w_a = 1/10 w_c$ and refractive index $\alpha = 3.53\text{-}i\gamma$. This resonator is sandwiched between two identical DBRs made of N pairs of dielectric layers of GaAs and Ga0.8Al0.2, where the latter material has refractive index $\alpha_L = 3.08$, with thicknesses $w_H = 79.36$ nm and $w_L = 69.48$ nm, respectively.

Note that in Fig. 2 (a) we show a part of the plane (κ, γ) where the stars mark the LEP eigenvalues for the resonator without DBRs and the thick dots mark the same for the resonator with two DBRs made of 20 pairs of layers each. The presence of reflectors is almost not change the normalized frequency of emission however the threshold gain of the mode experiences a drastic change if the frequency lays in the stop band of DBR. Namely, the threshold gain of the mode E_{11} drops from 0.7 to $2 \cdot 10^{-4}$ if the number of the pairs of layers in each DBR grows from 1 to 20. The computed LEP eigenvalues are found to satisfy the Optical Theorem with machine precision.

In Chapter 3, we analyze the properties of the infinite grating consisting of dielectric or quantum nanowires in the free space. At first, we study the problem of the scattering of plane waves, which are incident normally on such grating (see Fig. 3) assuming that the wire material is a lossless dielectric with refractive index

α. Then we study the LEP where $\nu = \alpha - i\gamma$. Here, two polarizations, *E* and *H*, should be studied separately with the aid of a scalar function $U(x, y)$, which is either E_z or $Z_0 H_z$ component of electromagnetic field, respectively. This function must satisfy the Helmholtz equation with different coefficients: $k^2\alpha^2$ or $k^2\nu^2$ inside the wires and k^2 outside of them. The field periodicity condition, $U(x + p, y) = U(x, y)$ enables us to reduce each of considered problems to elementary strip of the width *p* along the *y*-axis.

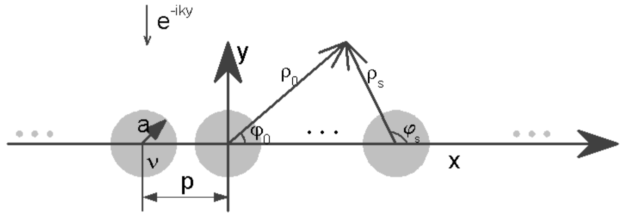


Fig. 3. Cross-sectional view of an infinite grating made of identical circular dielectric or quantum nanowires.

With the aid of separation of variables in local polar coordinates and the addition theorem for cylindrical functions, the plane wave scattering problem is reduced to a set of linear algebraic equations, which can be compactly written as the following operator equation:

$$[I + A(\sigma; \xi, \alpha)]X = Y, \quad I = \{\delta_{mn}\}, \quad A = \{A_{mn}\}_{m.n=-\infty}^{\infty}, \tag{2}$$

where $\sigma = p/\lambda$ is the normalized frequency, $\xi = p/a$ is the normalized distance between wire centers, $Y = \{y_m\}_{m=-\infty}^{+\infty}$ is a known excitation vector, $X = \{x_m\}_{m=-\infty}^{+\infty}$ is the vector of unknowns, and δ_{mn} is the Kroeneker delta.

Here, the matrix A_{mn} belongs to the Fredholm second kind type. Therefore the numerically obtained solution to (2), $\{x_m\}_{m=-N}^{+N}$, converges to exact solution by the norm in l_2 with larger truncation numbers *N*. Floquet harmonics, which enable one to build the field in the far zone of the grating, are obtained from computed $\{x_n\}$ using the Poisson transformation.

It is also necessary to note that the integer values of the normalized frequency, $\sigma = 1,2,3...$, correspond to the branching points of the field as a function of the wavelength λ; these points are called Rayleigh anomalies.

Color maps (reliefs) of the absolute value of the reflection coefficient of the plane wave by a grating of dielectric nanowires with $\alpha = 1.4142$ as a function of the normalized frequency σ and the normalized distance ξ (Fig. 4 (a)) show a number of maxima of reflection (bright "ridges"). They are caused by the resonances on the natural modes of various types that exist in the given periodic resonator. These resonances shift in frequency if the parameters ξ or α vary.

As known, the eigenvalues coincide with the poles of the resolvent of the scattering problem or, equivalently, with the roots of determinantal equation,

$$\det[I + A(\kappa, \gamma; \xi, \alpha)] = 0, \quad A = \{A_{mn}\}_{m.n=-\infty}^{+\infty}. \tag{3}$$

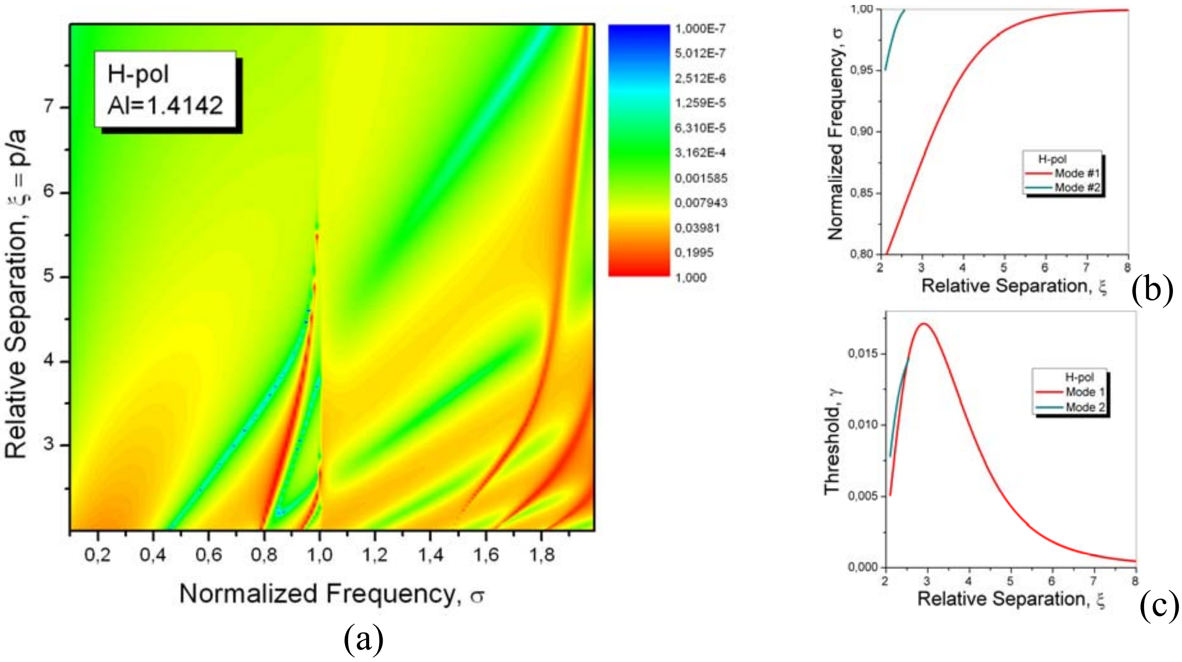


Fig. 4. Color maps of the absolute value of the reflection coefficient of the H-polarized plane wave from the grating of dielectric nanowires as a function of the normalized frequency σ and the normalized distance between the wires ξ at $\alpha = 1,4142$ (a). Dependences of the frequencies (b) and thresholds (c) of the grating modes on the normalized distance.

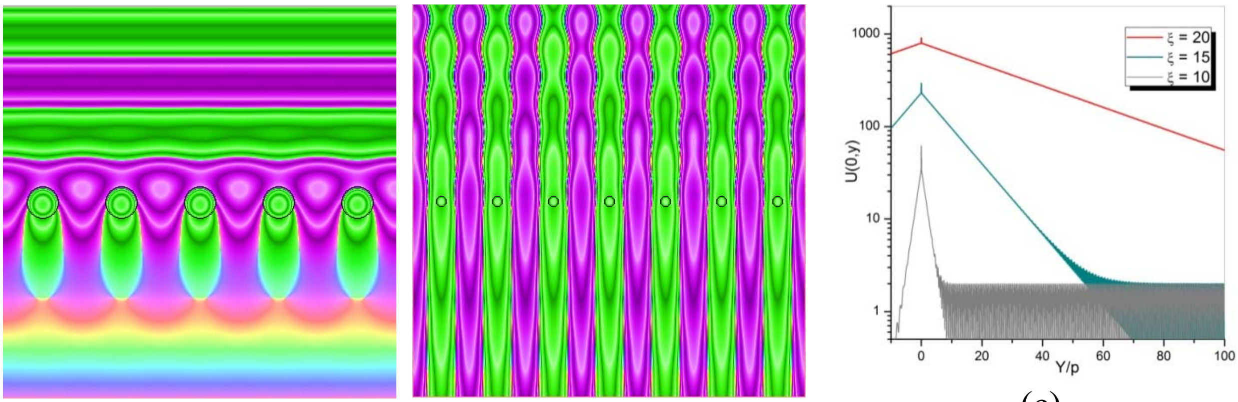
These roots can be classified to two classes. The first is the eigenvalues of the inner domain of each nanowire that are close to the zeros of one of the characteristic functions of a single dielectric wire,

$$F_m^{E,H} = \alpha^{\pm 1} H_m^{(1)}(ka) J_m'(\alpha ka) - H_m^{(1)\prime}(ka) J_m(\alpha ka), \tag{4}$$

where $m = 0,1,2,...$, and the functions involved are the Bessel and Hankel functions and their derivatives, however slightly shifted because of the coupling with all other wires. The corresponding to them maxima of reflection have the shape of broad ridges, which cross the vertical lines corresponding to the Rayleigh anomalies in Fig. 4 (a), with growing ξ, because for these roots $ka \approx const$ or $\sigma_{m,n}^H \approx const \cdot \xi$. We call them the modes of the nanowire of the type $H_{m,n}$.

The second class is the eigenvalues, for which the maxima on the maps in Fig. 4 (a) do not cross the mentioned vertical lines but tend to them with growing distance between the wires, ξ. This means that the corresponding to them poles of the resolvent tend to the branching points as $\sigma_{m,n}^{GH} \approx m - const \cdot \xi^{-q}$ $(q \geq 2)$ if $\xi \to \infty$. These natural modes are called the grating or lattice modes, $GH_{m,n}$.

Further we consider the LEP where there is no incident wave and the refractive index is assumed complex, $\nu = \alpha - i\gamma$ (with a known α). Then the mode



(a) (b) (c)

Fig. 5. The field in the grating-mode resonance GH_1^+ near the grating of dielectric nanowires ($\alpha = 2,46$) for the normally incident H-polarized plane wave: (a) $\xi = 5$, $\sigma = 0.776658$, on five periods, and (b) $\xi = 10$, $\sigma = 0.9967$, on seven periods. The cuts of the resonance field along the *y*-axis for three values of ξ (c)

threshold of self-excitation γ is sought for, together with the mode natural frequency σ, as an eigenvalue.

In Fig. 4 (b) and (c), we show the dependences of the frequencies and thresholds of two lowest grating modes of different symmetry across the line $y = 0$: GH_1^+ and GH_1^- on the normalized distance between the quantum wires, ξ. As one can see, if ξ gets larger, then the normalized frequencies of these modes tend to the Rayleigh anomaly at $\sigma = 1$. Still more important is the fact that the thresholds of self-excitation of the grating modes go to zero. This behavior is drastically different from the thresholds of the nanowire modes that remain finite and rather large if the wires have smaller than the wavelength diameter.

In Fig. 5, we present the field near the grating in the resonance on one of the grating modes, for the plane wave incident normally on the grating of dielectric nanowires with refractive index $\alpha = 2,46$ and several values of ξ. If $\xi = 5$, (Fig. 5 (a)), then the field maxima are on the wires and their values are a few times larger than the incident-wave amplitude. Fig. 5 (b) demonstrates the resonance on the same mode at $\xi = 10$, and the field maxima are exactly on the nanowires and in the middle between them that is the signature of the grating mode. The size of the domain (counted in periods) where the resonance field has large amplitude is shown in Fig. 5 (c). Here, we plot the cuts of the field along $x = 0$ for three values of $\xi = 10, 15, 20$ on the frequencies of the maxima of reflection.

In the first case the field maxima are approximately 60 times larger then the incident field, and the area of high intensity spreads to the distance of 8 periods. If $\xi = 15$ and 20, then the field maxima reach 300 and 1000, and the area of high field intensity spreads to 60 and 200 periods, respectively.

Using the Gershgorin theorem, we derived asymptotic expressions for the frequencies σ and threshold gains γ of the grating modes. For instance, for such mode of the first order, GH_1^+, if $\xi \to \infty$ or $\alpha \to 1$, then

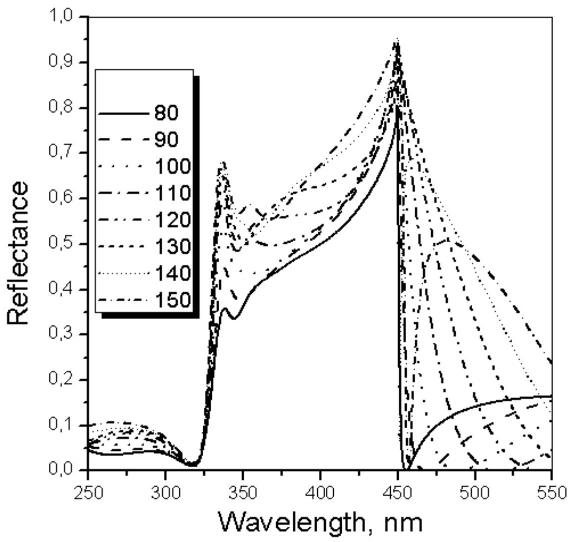
$$\sigma = 1 - 1/2\pi^8\left(\alpha^2 - 1\right)^2 \xi^{-8}, \quad \gamma = 1/8\pi^4(\pi - 1)\alpha\left(\alpha^2 - 1\right)^2 \xi^{-4}. \tag{5}$$

These asymptotic expressions confirm the mentioned above properties of the grating modes and show in detail how the corresponding to them eigenvalues tend to Rayleigh anomalies.

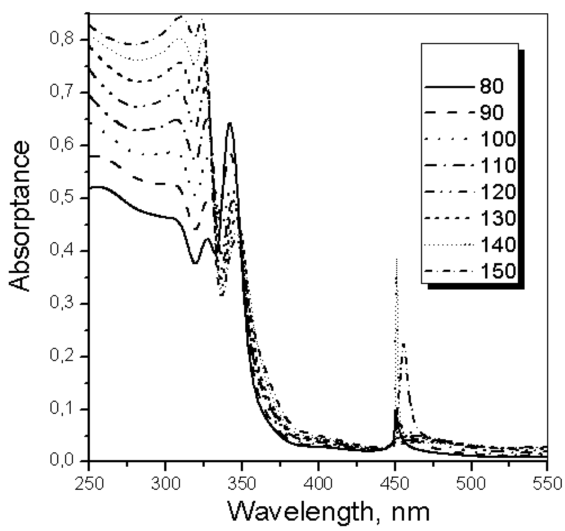
In Chapter 4, we study the effects that appear on the wire gratings in the presence of nanowires made of noble metals, in the visible range. At first, we analyze the scattering of light on an infinite grating of silver nanowires in the free space; then we continue this analysis to a binary grating made of both dielectric and silver nanowires. After that we study the LEP eigenvalues connected to the surface-plasmon modes and the grating modes (caused by the periodicity) of a binary grating made of silver and quantum nanowires.

In Fig. 6, we show the plots of the absolute value of the reflectance and absorbance of the H-polarized plane wave normally incident on the grating of silver nanowires of the radius $a = 80, 90, \ldots 140, 150$ nm and period $p = 450$ nm. One can see a sharp resonance near to $\lambda = 450$ nm that equals to period: this is the resonance on the grating mode. The other resonance is seen at the wavelength $\lambda \approx 348$ nm that corresponds to the root of equation $\varepsilon(\lambda) = -1$, which is the asymptotic form of equation (4) if $ka \ll 1$, $m \geq 1$. This is the localized surface-plasmon resonance. It is interesting by the fact that its frequency is almost independent of the radius of nanowires if $a \ll \lambda$.

It should be noted that the analysis of plasmonic effects in the context of a lasing for such a configuration has not been performed so far.



(a)



(b)

Fig. 6. Absolute value of the reflectance (a) and the absorbance (b) of the plane wave incident normally on the grating of silver nanowires with period 450 nm and the radius varying from 80 nm to 150 nm.

In this thesis, we study a binary grating made of quantum and silver nanowires (Fig. 7). The color maps of reflectance and absorbance are shown in Fig. 8 (a) and (b) in dependence on the wavelength and the angle of positioning of the wires ϕ, for the wires of identical radius, $a_1 = a_2 = 50\,\text{nm}$, placed at the distance of 100 nm from the local origin at $\phi_1 = \phi$ and $\phi_2 = \pi + \phi$.

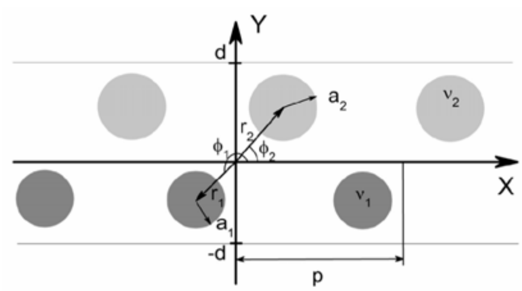


Fig. 7. Cross-sectional view of an infinite binary grating of circular nanowires made of silver and dielectric, i.e. having different refractive indices

As visible, the wavelength band of high reflection between the surface-plasmon and the grating-mode resonances remains approximately the same for all values of the angle ϕ. The resonances on the grating modes show up, on the maps of reflectance and absorbance, as two "ridges" slightly to the right from the wavelength $\lambda = p$. Note

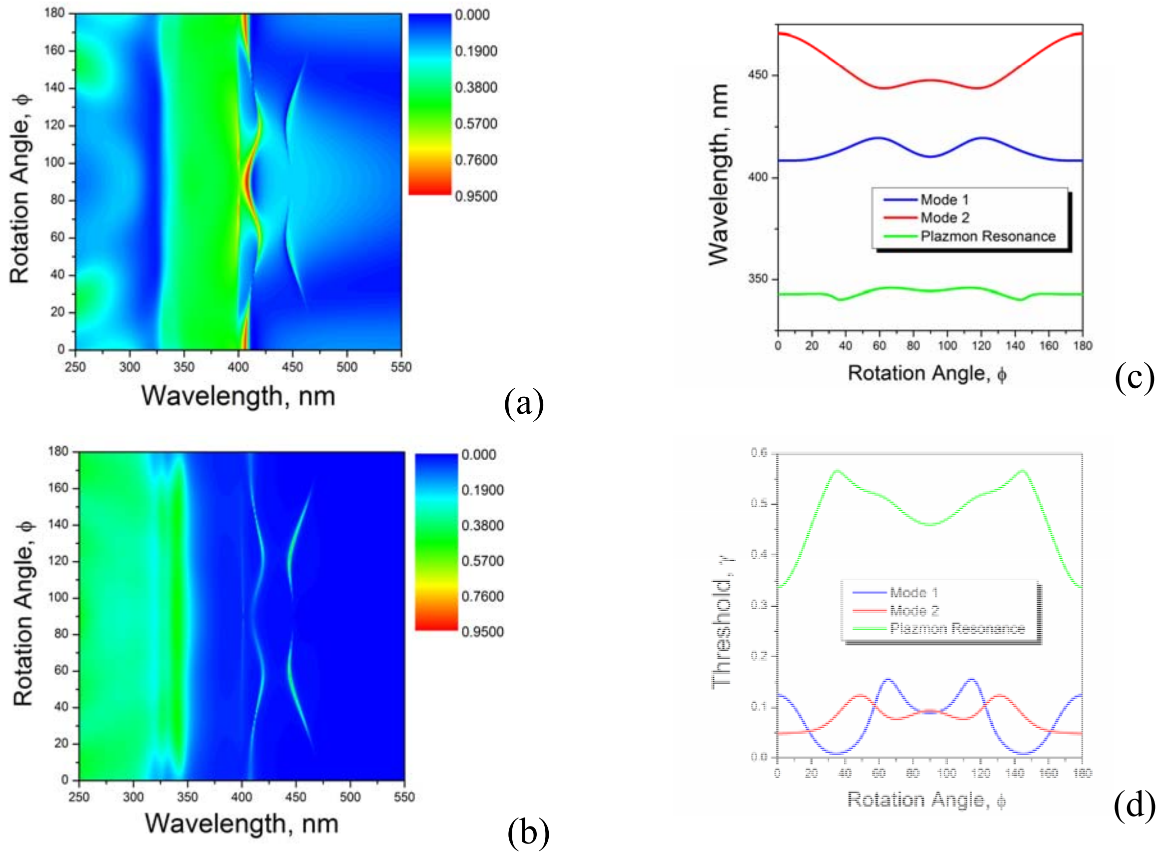


Fig 8. Color maps of the absolute value of reflectance and (a) and absorbance (b) as a function of the angle of positioning of wires and the wavelength for the H-polarized plane wave normally incident on the binary grating of dielectric and silver nanowires with period $p = 400\,\text{nm}$ and radius $a_1 = a_2 = 50\,\text{nm}$ and refractive index $\alpha = 2.48$; wire center coordinates are $r_1 = r_2 = 100\,\text{nm}$ and $\phi_1 = \phi$, $\phi_1 = \phi + \pi$. The wavelengths (c) and threshold gains (d) of the lasing modes as a function of the angle of positioning in the binary grating.

that these “ridges” vanish near to $\phi = 0, \pi/2$ and π, i.e. if the wires form configurations with two lines of symmetry. This can be explained by the fact that the natural fields of these modes are anti-symmetric with respect to the y-axis and hence cannot be excited by the normally incident plane wave.

To make a comparison between the surface-plasmon mode and the grating modes, we compute the variation of the LEP eigenvalues with the rotation of the pair of wires around the center of the distance between them in the elementary cell. Fig. 8 (c) and (d) show the dependences of eigenvalues on the angle of positioning for three different modes of the same grating as in the plane-wave scattering problem demonstrated in Fig. 8 (a) and (b).

As before, the resonance wavelength enables us to identify easily the modes: the surface-plasmon mode remains close to $\lambda \approx 340$ nm while two other modes are the grating modes because their wavelengths are slightly larger than $\lambda = p = 400$ nm. Note that the first and the second grating modes appear on the color maps in Fig. 8 (a) and (b) as narrow bright ridges while the surface-plasmon mode is visible as a wide strip. AS could be expected, the dependences of the lasing wavelength on ϕ have almost the same form as the ridges of high-Q resonances in Fig. 8 (a) and (b). The threshold gain of the grating mode 1 has a minimum for the vertical arrangement of wires ($\phi = \pi/2$). However a deeper minimum is observed if the wires are placed at the angle of approximately 45^{o} in the elementary cell.

This can be explained taking into account the areas of high intensity of the electric field of the grating mode made of silver wires. Indeed, the natural magnetic field of the grating mode that is symmetric along the *x*-axis has large maximum in the middle between the wires. As known, the natural electric field has zeros at the same places where the magnetic field has maxima. Therefore placing a quantum wire in the middle between the silver wires leads to inefficient overlap between the active region and the electric field of mode 1 and, hence, to high threshold. If $\phi = \pi/2$, then the mode 2 has the opposite symmetry along the *y*-axis with respect to the mode 1, therefore its threshold behaves differently – see Fig. 8 (b). Note also that mode 1 and 2 display hybridization (also called parametric interaction) at the variation of the angle ϕ: their frequencies get near at the values of ϕ where the thresholds cross each other.

The most valuable result of this study of the lasing modes of a binary grating, as we believe, is the finding that the threshold gain of the grating mode can be from 3 to 60 times lower than the threshold gain of the surface-plasmon mode, at least if all silver and quantum wires have the same radii of 50 nm.

In Chapter 5, we study the properties of the infinite gratings made of dielectric, metallic and quantum nanowires located in a flat-layered host medium. This choice is related to the consideration that frequently in realistic circumstances the gratings of nanowires are manufactured in such a way that the wires are embedded into a “matrix”, i.e. a flat dielectric layer of different refractive index.

One of such periodic structures is shown in Fig. 9: this is a dielectric layer with refractive index α_S and thickness d. Inside this layer there is an infinite grating made of dielectric wires placed at the distances d_1 and $d_2 = d - 2a$ from the lower and upper boundaries of the layer, respectively. The period of the grating is p, the wire radius is a, and its refractive index is α in the plane-wave scattering problem and $\nu = \alpha - i\gamma$ in the LEP.

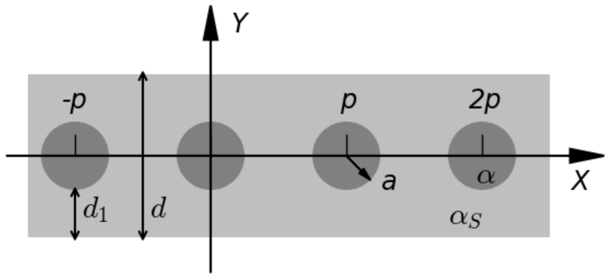
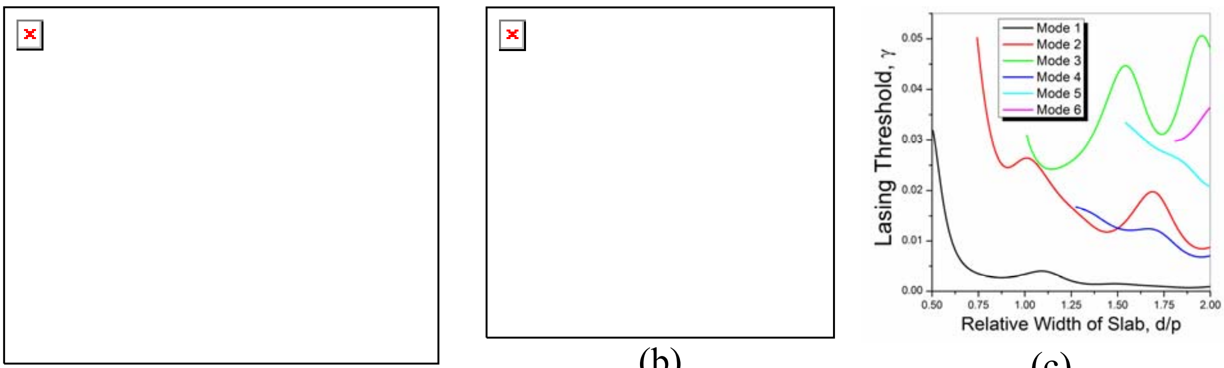


Fig. 9. Cross-sectional view of an infinite grating of circular nanowires placed into a flat dielectric layer

The treatment of electromagnetics problems is based on the use of the scattering matrix approach. For building the scattering matrix of a layer with a wire grating, one has to multiply the scattering matrices, in terms of the Floquet harmonics, of the grating itself and of the flat boundaries, and also the matrices of the plane wave propagation through uniform dielectric layers of thicknesses $d_{1,2}$.

In Fig. 10 (a), we present the color map of the absolute value of the reflectance of the normally incident H-polarized plane wave as a function of normalized thickness and the normalized by the period frequency σ. The grating period, denoted as p, is fixed to be $4a$, the refractive index of the layer is $\alpha_S = 1{,}6$ and the refractive index of the wires is $\alpha = 2$. The ratio of the layer thickness to the period varies from 0.51 to 2. Here, the smallest value of d/p corresponds to the case of the thickness being only slightly larger than the wire diameter, and the largest value corresponds to $d = 2p$. One can see two types of resonances on this color map, each of them showing up as a curved ridge.



(a) (b) (c)

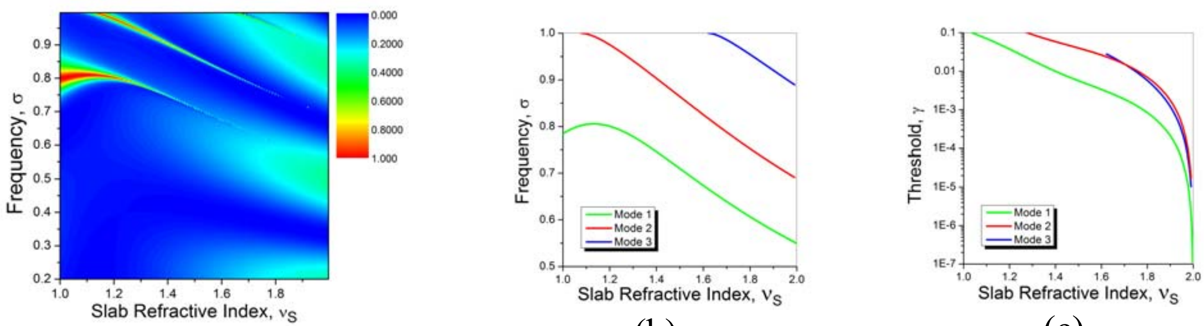
Fig. 10. Color map of the absolute value of the reflectance (a) as a function of the relative thickness of the layer with refractive index $\alpha_S = 1{,}6$ and the normalized wavelength, for the plane H-wave normally incident on the grating with period $p = 4a$ made of the dielectric wires with $\alpha = 2$. Frequencies of emission (b) and threshold gains (c) for the same configuration as a function of the normalized layer thickness.

The first type is the relatively broad and low ridges, which correspond to the low-Q resonances on the dielectric layer modes. The second type is the sharper and higher ridges, which correspond to the high-Q grating modes of the wire grating.

It is worth noting that the growth of the layer thickness leads to appearance of the grating modes of higher orders. The dependences of the grating-mode frequencies and associated thresholds on the normalized layer thickness are shown in Figs. 10 (b) and (c). They demonstrate good agreement between the resonance frequencies in the plane-wave scattering problem and the frequency of self-excitation in the laser problem. As for the thresholds, their behavior is determined by the overlap coefficients between the quantum wires and the electric field of the working mode.

Consider now the dependence of the LEP eigenvalues for the grating modes on the refractive index of the layer. Here, we assume that the refractive index of the wires is $\alpha = 2$. The wire grating is placed in the middle of the layer, so that $d_1 = d_2 = d - 2a$, the layer thickness equals to the period, $d = p$, and the refractive index of the layer varies from 1 to 2. This variation corresponds to the transformation of the structure from a dielectric wire grating in the free space to a uniform dielectric layer with refractive index $\alpha_S = \alpha = 2$ in the free space. In the intermediary situations, we have a flat dielectric layer with embedded wire grating having a refractive index larger than the layer. In Fig. 11 (a), we present the color map of the absolute value of the reflectance of such a structure in the case of the H-polarization. As mentioned, the right boundary of the map corresponds to the uniform dielectric layer; the cut of the map along that line shows sinusoidal dependence, which is the same for either polarization because of the normal incidence. The broad ridges that start here are the resonances on the layer modes. The resonances on the grating modes stretch from the left boundary of the same map as sharp narrow ridges. The smaller the contrast between the refractive indices of the layer and the wires, the narrower the latter ridges.

The corresponding dependences of the LEP eigenvalues of the grating



(a) (b) (c)

Fig. 11. Color map of the absolute value of reflectance as a function of the refractive index of layer α_S and the wavelength of the plane wave normally incident on the grating of the period $p = 4a$ made of dielectric wires with $\alpha = 2$ (a). Frequencies (b) and threshold gains (c) of the same modes for the grating of quantum wires in a flat layer, H polarization

modes of the grating of quantum wires embedded into the passive layer are shown in Fig. 11 (b) and (c). The plots of the frequencies of emission fully agree with the resonance ridges on the map of the reflectance. The plots of the thresholds demonstrate important result: if the contrast between the refractive indices of the layer and the wires is getting lower, the thresholds rapidly drop. This fact is in agreement with results presented in Chapter 3 where we consider a grating of quantum nanowires with small refractive index in the free space.

Conclusions

In the thesis, we have studied a timely problem of electromagnetics that consists of development of linear electromagnetic model able to characterize the frequencies and the thresholds of self-excitation of the natural electromagnetic fields (modes) of periodic open resonators made of circular dielectric and metal nanowires, with active regions made of quantum wires. In the framework of such model, we have studied the modified for lasers eigenvalue problem for several important configurations of two-dimensional periodic resonators. Among them, there is an infinite grating of quantum nanowires in the free space or in a flat-layered medium and a binary grating made of quantum and silver nanowires. As auxiliary problems, we have considered the scattering and absorption of plane waves of two polarizations by the mentioned above gratings.

The main scientific and practical results are as follows:

- The electromagnetic characteristics have been obtained of the so-called grating modes, the frequencies of which are close to the Rayleigh anomalies, of periodic open resonators made of nanowires.
- It has been established that in the infinite grating of thin quantum nanowires the grating modes can have arbitrarily low thresholds of self-excitation; these thresholds can be lowered by making larger the distance between the wires, making lower their refractive index, and placing them between the distributed Bragg reflectors.
- It has been found that in the visible range the spectra of the scattering and absorption of waves by a grating of metal nanowires and by a binary grating of dielectric and metal nanowires demonstrate co-existing resonances on the surface-plasmon modes and on the grating modes.
- It has been demonstrated that for the binary grating of quantum and metal nanowires the thresholds of self-excitation of the grating modes can be considerably lower than those of the plasmon modes.
- The Poynting theorem has been derived for the natural modes of a periodic open resonator of quantum wires that links the mode threshold gain to the mode field characteristics.
- The asymptotic expressions have been derived for the complex natural frequencies of the grating modes of the grating made of circular dielectric nanowires and for the thresholds of such modes of the grating of circular quantum wires having small radius or small optical contrast with the host medium.

List of the main publications related to the thesis

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2. V. O. Byelobrov, J. Ctyroky, T. M. Benson, A. Altintas, R. Sauleau, A. I. Nosich, "Low-threshold lasing modes of an infinite periodic chain of quantum wires," *Optics Letters,* vol. 35, no 21, pp. 3634-3636, 2010.
3. E. I. Smotrova, V. O. Byelobrov, T. M. Benson, J. Ctyroky, R. Sauleau, A. I. Nosich, "Optical theorem helps understand thresholds of lasing in microcavities with active regions," *IEEE J. Quant. Electron.*, vol. 47, no 1, pp. 20-30, 2011.
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5. V. O. Byelobrov, T. M. Benson, A. I. Nosich, "Binary grating of sub-wavelength silver and quantum wires as a photonic-plasmonic lasing platform with nanoscale elements," *IEEE J. Selected Topics Quantum Electronics,* vol. 18, no 6, pp. 1839-1846, 2012.
6. V. O. Byelobrov, T. M. Benson, "Extraordinary high-Q resonances in the scattering by a dielectric slab containing a grating of circular cylinders," *International Journal Semiconductor Physics, Quantum Electronics, and Optoelectronics,* ISP NASU Press, Kiev, vol. 17, no 1, pp. 100-105, 2014.
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8. T.L. Zinenko, V.O. Byelobrov, M. Marciniak, J. Ctyroky, A.I. Nosich, "Grating resonances on periodic arrays of sub-wavelength wires and strips: from discoveries to photonic device applications," in O. Shulika, I. Sukhoivanov (Eds.) *Contemporary Optoelectronics: Materials, Metamaterials and Device Applications,* Springer Ser. Optical Sciences, vol. 199, pp. 65-79, 2016.
9. V. O. Byelobrov, T. M. Benson, A. I. Nosich, "Near and far fields of high-quality resonances of an infinite grating of sub-wavelength wires," *Proc. European Conf. Microwaves (EuMC-2011)*, Manchester, 2011, pp. 858-861.
10. V.O. Byelobrov, T.M. Benson, A.I. Nosich, "Plasmon resonances of an infinite grating of silver wires coated with dielectric envelopes," *Proc. Int. Conf. Transparent Optical Networks (ICTON-2012)*, Coventry, 2012, Tu.A5.6.

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Full list of publications can be seen at http://ire.kharkov.ua/LMNO/volodya.html