INTRODUCTION

This work deals with research, using boundary-value problems for the Maxwell equations, into electromagnetic fields, frequencies and thresholds of lasing for the eigenmodes of stand-alone and coupled dielectric resonators with active regions.

Timeliness of research. Development of devices and systems that use electromagnetic waves for transmitting and processing the information heavily relies on the availability of small-size and efficient sources of short waves, from THz to the visible to UV. Today one of the key sources in these wave bands is semiconductor, crystalline and polymeric microcavity lasers. Such lasers, frequently shaped as thin disks, are equipped with active regions and pumped either with photo-pumping or with injection of carriers from metallic electrodes. In particular, such devices are considered now as the most promising sources of THz waves; they are also viewed as potential sources of single photons for the future quantum computer. Design and manufacturing of these lasers depends on complicated technologies such as dry and wet etching and molecular-beam epitaxy, and their measurements require fine spectroscopic equipment. Today there exist only several major laboratories that manufacture and measure microcavity lasers: for instance, Caltech, Yokohama National University, Laboratory of Photonics and Nanostructures of CNRS in Marcoussi, Federal Polytechnic University of Zurich, and Institute of Semiconductors of the Chinese Academy of Sciences. Therefore, it is clear that preceding modeling of such expensive devices and adequate theoretical description of the associated physical effects are critically important elements of successful research and development in this field.

However, the approaches and methods of linear modeling of microcavity lasers so far have been based exclusively on the search of complex-valued natural frequencies and associated modal fields in the *passive* dielectric resonators. Here, two approaches have been most widely used: geometrical optics (GO), known also as the billiards theory, and numerical method of finite differences in time domain (FDTD). Despite their simplicity and usefulness, each of them suffers of a number of heavy demerits. GO is not applicable to the cavities whose dimensions are comparable to the wavelength and is not able to estimate the losses and therefore the Q-factors of modes. Moreover, GO cannot grasp the discreteness of the modal spectrum of open resonator. FDTD cannot access the natural modes directly. It needs a pulsed source placed in the cavity, calculates the transient response to that source at some other point, implies the use of Fourier transform to obtain frequency dependence, and finally restores the Q-factors from the widths of resonant peaks. All this involves multiple uncontrollable errors and generally cannot guarantee the desired accuracy of modeling.

The most fundamental defect of the conventional approach is the fact that in the passive model one ignores the presence of active region. As a result, there is no chance to reproduce and quantify such a fundamental property of laser as existence of lasing threshold or explain why the light emission frequently occurs on the modes that do not possess the highest Q-factors in the absence of pumping. The attempts of building the theory able to deliver the thresholds have been linked to the quantum-mechanical nonlinear models and have not been based on the "first principles', which are the Maxwell equations with accurate boundary conditions and condition of radiation. Therefore the area and the topic of the undertaken research are timely

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

1. Government R&D projects of IRE NASU, "Theoretical and experimental investigation of wave processes in the devices and components of microwave and millimeter-wave bands" (code Buksir-2, #01.00U006441, 2002-2006) and "Development and application of new methods of computational radio-physics, theoretical and experimental investigation of transformations of electromagnetic

fields of the GHz and THz bands in the objects and media of anthropogenic and natural origin" (code Buksir-3, #01.06U011975, 2007-2010).

2. Program of NASU "Nanostructured systems, nanomaterials and nanotechnologies" via competitive project "Micro and nanoscale electromagnetic modeling of optical fields in resonators with active regions shaped as quantum layers, wires and dots" (code Porig, # 01.07U003983, 2007-2009).

3. Competitive project of the Ministry of Education and Science, Ukraine "Innovative numerical modeling of quasioptical focusing systems" (code Fokus, # 01.09U005351, 2009-2010)

4. Exchange program between NASU and the Royal Society, UK via joint projects «Modeling of micro and nano-scale resonators and lenses for dense photonic circuits» (#IJP-2004/R1-FS, 2004-2007) and «Advanced modeling of single and periodic active dielectric resonators for microlasers» (#IJP-2007/R1, 2007-2009) with the University of Nottingham.

5. Exchange program between NASU and TUBITAK via joint project «Innovative electromagnetic modeling of multielement quasioptical focusing systems for sub-mm and terahertz ranges» (#106E209, 2007-2009) with the Bilkent University, Ankara.

6. Exchange program between NASU and the Academy of Sciences of Czech Republic (ASCR) via joint project «Electromagnetic and numerical modeling of active and nonlinear microcavities» (2008-2010) with the Institute of Photonics and Electronics of ASCR, Prague.

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

- "Eigenvalue problems for cyclic photonic-molecule microcavity lasers," IEEE Electron Devices Society (2005),

- "Quasi-3D electromagnetic modeling of microcavity lasers and laser arrays with lowered thresholds and improved directionalities," INTAS association, EU jointly with the University of Nottingham, UK (2005-2007),

- "Advanced linear modeling of semiconductor microcavity lasers," International Visegrad Fund, EU jointly with IPE ASCR, Prague (2007-2008),

- "Electromagnetic modeling and design of dielectric lenses and resonators for the emerging photonic and THz applications," Ministry of Foreign and European Affairs, France jointly with the University of Rennes 1, Rennes (2008-2009).

Aims and tasks. The aims of research in the thesis are the building of the linear model to study the natural electromagnetic fields (modes) in the stand-alone and coupled two-dimensional (2-D) dielectric resonators with active regions, development on its basis of the numerical algorithms, computation of spectra of emission and associated thresholds for the modes in certain important types of resonators, and formulation of recommendations towards reduction of thresholds and improvement of directionality of radiation. To achieve these goals, the following problems have been considered:

- Formulation of the mathematical problem for adequate description of the natural electromagnetic fields (modes) in open resonators with active regions,
- Development of numerical algorithms for the computation of frequency spectra and thresholds of lasing, and also modal fields in the near and far zones,
- Systematic computation of the frequencies and thresholds of lasing and modal fields for the following resonator configurations:

- stand-alone circular resonators including a uniformly active one and a resonator with a partial (radially inhomogeneous) active region,

- active disk in a passive ring and an annular Bragg reflector,

- cyclic photonic molecules made of active circular disks,

- stand-alone active resonator with the spiral contour.

The object of research in the thesis is the effect of radiation of monochromatic electromagnetic waves from stand-alone and coupled dielectric resonators with active regions.

Specifically, we study the natural electromagnetic fields in two-dimensional (2-D) models of stand-alone and coupled dielectric resonators with active regions and their spectra of natural frequencies and associated material thresholds.

Methods of research used in the thesis are the following: theory of boundary-value problems of electromagnetics that views the natural modes as the solutions to the homogeneous time-harmonic Maxwell equations with rigorous boundary conditions and radiation condition at infinity. Dimensionality of these problems is reduced to 2-D using widely known approximate method of effective refractive index. For each of considered configurations, the obtained 2-D problems are equivalently reduced to homogeneous matrix equations of the Fredholm second kind. For the stand-alone and uniform and layered circular resonators and made of them photonic molecules this is achieved by using the full or partial separation of variables. For the resonator with arbitrary smooth contour the same is achieved by using the method of the Muller boundary integral equations discretized with a Nystrom-type interpolation algorithm. The eigenvalues as the roots of corresponding determinantal equations are found numerically with controlled accuracy using two-parametric iterative Newton algorithm.

Scientific novelty of obtained results is determined by the following considerations:

- The problem of natural modes of open dielectric resonators has been formulated, for the first time, in such a manner that takes into account the presence of active region and, as a result, enables one to find the modal frequencies and associated thresholds of lasing.
- For the first time an analytic connection has been found between the threshold of lasing and the mode Q-factor and the overlap coefficient between the active region and the mode electric field.
- It has been established that in a stand-alone circular disk there exist lower-order modes with high thresholds of lasing and the whispering-gallery modes with exponentially low thresholds.

- It has been shown, for the first time, that one can lower the thresholds of lasing of supermodes (coupled modes) built either on the lower-order modes or on the whispering-gallery modes by collecting the disks into a cyclic photonic molecule.
- It has been found, for the first time, that the threshold of lasing of any supermode in an active disk placed inside a passive annular reflector can be both lower and higher than in a stand-alone disk. This depends on the field overlap with the active region: the threshold greatly increases if the field is pulled into passive regions.
- It has been quantified how the deformation of the disk to a spiral resonator leads to the splitting of the modes to doublets. Here, the directionality of emission of the whispering-gallery modes improves however their thresholds grow up. The main factor is the height of the step on the contour in terms of mode wavelength.

Practical importance of obtained results. The proposed approach and the developed numerical algorithms can be used in the electromagnetic analysis of lasing modes of microresonator lasers of the UV, visible, IR, and THz ranges shaped as thin disks, cyclic photonic molecules of such disks, disks in the annular Bragg reflectors, and also thin active resonators with arbitrary contours. The established properties of the modes in such resonators significantly deepen our understanding of the thresholds of lasing. They also show the ways to the lowering of the thresholds and improving the emission directionality. Currently it is planned that some of the predicted effects will be looked for experimentally at the Ecole Normale Supeieur de Cachan, France where stand-alone and coupled polymeric microresonator lasers are studied.

Personal contribution of the candidate. All main results presented in the thesis belong to the author. Her contribution, in the co-authored papers [1-5,7-13], is in the derivation of the basic equations, development of numerical algorithms, systematic computing of the lasing frequencies and thresholds, and interpretation of numerical results; in the review paper [6] it consists of computations of sample dependences illustrating the behavior of lasing thresholds for the modes of circular resonators and photonic molecules.

Dissemination of the results. The results of this thesis have been personally presented by the author at the following scientific seminars: “Computational electromagnetics” at IRE NASU (Prof. A.A. Kirilenko), “Integral equations of electromagnetics” at the Kharkov National University of Radio Electronics (Prof. A.G. Nerukh), at the Department of Electrical and Electronics Engineering of the Bilkent University, Ankara (Prof. A. Altintas), at the George Green Institute for Electromagnetics Research of the University of Nottingham, UK (Prof. T.M. Benson), at the Photonics Research Group of the Aston University (Dr. V.K. Mezentsev), and at the Institute of Photonics and Electronics of ASCR, Prague (Prof. J. Ctyroky). They were also presented at the following national and international conferences:

- Days on Diffraction, St. Petersburg (2004, 2007)
- Physics and Engineering of Microwaves, Mm and Sub-mm Waves, Kharkov, (2004, Best Poster Paper Prize at the Young Scientist Contest)
- Mathematical Methods in Electromagnetic Theory, Dnipropetrovsk (2004)
- Antennas and Electromagnetics, Saint Malo (2005)
- Microwave and Optical Technologies, Fukuoka (2005, Invited Paper)
- Advanced Optoelectronics and Lasers, Alushta (2003,2008), Yalta (2005)
- Numerical Simulation of Optoelectronic Devices, Berlin (2005)
- Workshop on Electromagnetic Wave Scattering, Gebze (2006, Invited Paper)
- Mediterranean Microwave Symposium, Budapest (2007, Invited Paper)
- Nanosystems, Nanostructures and Nanotechnologies, Kiev (2007)
- Open Waveguide Theory and Numerical Modeling, Prague (2003), Grenoble (2005), Varese (2006), Copenhagen (2007), Eindhoven (2008)
- Transparent Optical Networks, Warsaw (2003), Wroclaw (2004), Barcelona (2005), Nottingham (2006), Rome (2007), Athens (2008), Ponta Delgada (2009)

- Waves in Science and Engineering, Mexico City (2009, Invited Paper)
- IX Young Scientists Conference on Radio Physics and Electronics, Kharkov (2009)

Publications. The results of research have been published in 46 papers including 8 papers in technical journals [1-8] and 38 papers in the proceedings and digests of international conferences [9-46].