LINEAR OPTICAL MODELING OF MICROCAVITY LASER MODES: THRESHOLDS, FREQUENCIES, DIRECTIVITIES

(Invited)

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***Abstract* – This paper 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 microcavity lasers.**

I. INTRODUCTION

Development of devices and systems that use electromagnetic waves for transmitting and processing information heavily relies on the availability of small-size and efficient sources of short waves, from THz to the visible to the ultraviolet range. Today one of the key sources in these wave bands is semiconductor, crystalline and polymeric microcavity lasers. Such lasers, frequently shaped as thin flat disks, are equipped with active regions and pumped either with photo-pumping or with injection of carriers from metallic electrodes [1-3]. 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. 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 method 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 not based on the “first principles,” which are the Maxwell equations with accurate boundary conditions and condition of radiation. This has been calling for the development of more adequate linear model of laser.

II. LINEAR MODEL OF MICROCAVITY LASER

Since 2003, we have been directing our research to creation of new 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 various 2-D resonators, and formulation of recommendations towards

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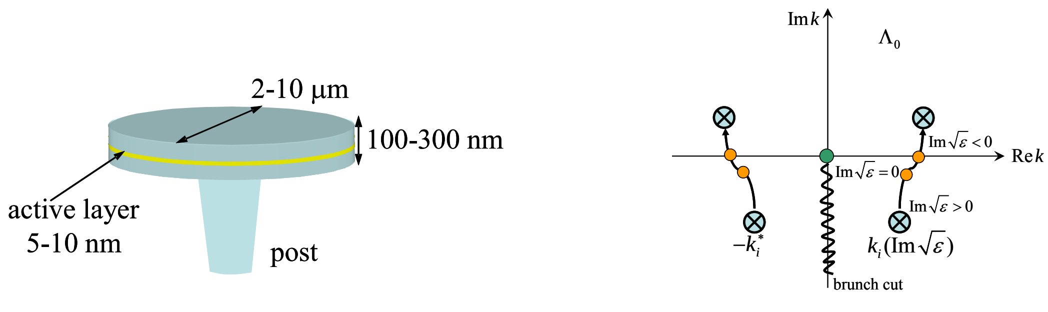
reduction of thresholds and improvement of directionality of radiation. More specifically, the following tasks have been considered:

- 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 off the frequencies and thresholds of lasing and modal fields for the following 2-D resonator configurations:

(i) stand-alone circular resonators including a uniformly active circle and a circular resonator with a partial (radially inhomogeneous) active region, (ii) active circle in a passive ring and an annular Bragg reflector, (iii) cyclic photonic molecules made of identical active circular cavities, and (iv) stand-alone active resonators with spiral, kite, and limacon contours.

As a general approach of our research, we have used the theory of boundary-value problems of electromagnetics, which imply that the natural modes are the solutions of the homogeneous time-harmonic Maxwell equations with rigorous boundary conditions and radiation condition at infinity. Dimensionality of these problems has been reduced from 3-D to 2-D using widely known approximate method of effective refractive index. For each of considered configurations, the obtained 2-D problems have been equivalently reduced to homogeneous matrix equations of the Fredholm second kind. For the stand-alone and uniform and layered circular resonators and photonic molecules of them this has been achieved by using the full or partial separation of variables. For the resonator with arbitrary smooth contour the same has been 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 have been searched for numerically with controlled accuracy using two-parametric iterative Newton algorithm.



(a) (b)

Fig. 1. (a) Sketch of the structure of a semiconductor microdisk laser of infrared band on a pedestal. (b) The trajectory of the eigenfrequency on the complex plane under the variation of the imaginary part of refractive index.

Microcavity lasers as open dielectric resonators with active regions first appeared in the 1990s as miniature semiconductor sources of infra-red waves [1]; later polymeric and monocrystal lasers were proposed for the visible, ultraviolet and terahertz bands. Usually they are shaped as circular disks having diameter of 10-20 wavelengths and thickness of 0.1-0.5 wavelengths, standing on a pedestal (Fig. 1 (a)) or laying on a less optically dense substrate. Inside the disk, there is a 5-10 nm thin active layer able to support the inversed population of carriers. For example, for semiconductor lasers it can be a thin quantum well, a layer of quantum dots, and also a cascade of such layers. For polymeric lasers, the whole disk becomes active under pumping.

The main properties of such lasers are the ultra-low thresholds of lasing, equidistant spectrum of lasing frequencies, and concentration of the radiation in the plane of the disk [1-3]. All these properties can be explained if the working modes of the disk laser are the whispering-gallery modes, whose fields are concentrated at the inner side of the disk rim. Today trends in the research into microdisk lasers are connected to the further lowering of the lasing thresholds and the improvement of the emission directionality. To achieve these goals, researchers work on smoothing the disk rim, optimize the shape and location of the active region (pumped area), integrate active disk into an annular Bragg reflector, collect the disks into photonic molecules, and also find optimal shapes of non-circular dielectric resonators.

In the modeling of passive thin flat dielectric resonators, first of all, there is an opportunity of approximate lowering of the dimensionality of the original 3-D problem to two dimensions, in the median plane of the disk, by using the so-called method of effective refractive index [4]. As it has been mentioned above, two most popular methods of the field analysis in dielectric resonators - GO and FDTD method - have certain important deficiencies. As these deficiencies cannot be eliminated, lately a growth of the publications using the methods of volume and boundary integral equations (IEs) has been observed. However, many types of the IEs are not fully equivalent to the original boundary-value problem, and thus possess a set of spurious eigenvalues. If a dielectric resonator is located in free space, then the spurious eigenfrequencies of such "defective" IE models are purely real. This seriously undermines the search for the true eigenfrequencies with small imaginary parts (high Q-factors). It is emphasized that there exists IE that is free from the mentioned defects. This is the set of the Muller boundary IEs – a pair (in 2-D) of coupled IEs with smooth or integrable kernels. The ways of efficient discretization of such IEs are discussed.

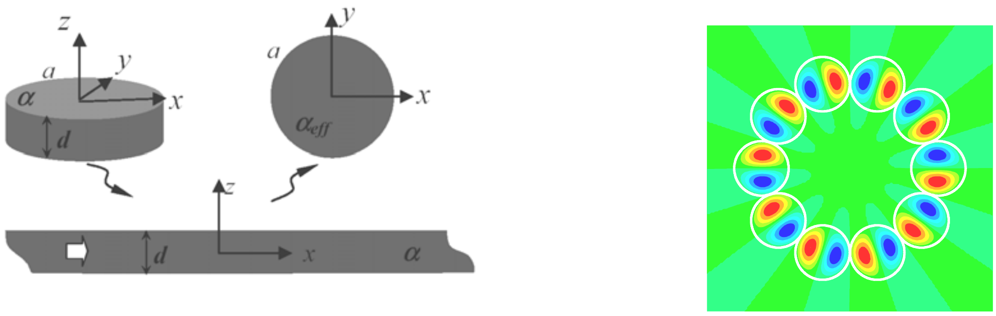
The opportunities and shortcomings of the model of passive dielectric resonator are discussed when applied to the investigation of lasers as open resonators with active regions. This analysis leads to the necessity of modification of the formulation of the eigenfrequency problem for a dielectric resonator. We have proposed to make use of the known description of the active (i.e. pumped) material as the one with negative losses. In line with the general theorems of operator-valued function analysis, each complex-valued eigenfrequency of a dielectric resonator is analytic function of the complex refractive index [5] (see Fig. 2). Here, for a passive dielectric resonator all eigenfrequencies are located strictly on one halfplane of the complex plane. However, if the imaginary part of refractive index becomes "active", then the eigenfrequencies are allowed to migrate to the other halfplane. For each mode the crossing of the real axis takes place for a specific value of the imaginary part of refractive index as spatially-averaged material gain. This value corresponds to the threshold of lasing as the process of emission of non-damped in time electromagnetic waves.

Therefore we have proposed to make the next step and look for the threshold value of the imaginary part of refractive index together with the real-valued emission frequency of a dielectric resonator mode as two elements of the same modified eigenvalue (see [3,6]). Here, it is necessary to demand the continuity of the field tangential components at the boundary of the active region. As the fields of the modes having real frequencies do not grow at infinity in space, for correct formulation of the problem one may use the Sommerfeld condition of radiation. We can also point out to a certain similarity between the proposed approach and a variant of the so-called method of generalized eigenoscillations, where the frequency was a known parameter and the eignevalues were sought for the complex-valued permittivity of a dielectric resonator [7].

III. 2D Models of Thin Circular Disk

When using the method of effective refractive index, it is assumed that homogeneous and isotropic disk of thickness d and radius a is located in free space. The real-valued bulk refractive index of disk material is denoted as α . It is assumed that electromagnetic field depends on time harmonically as $e^{-i\omega t}$ and free-space wavenumber is $k = \omega / c = 2\pi / \lambda$, where ω is the frequency, c is the free-space light velocity, and λ is the wavelength. The effective refractive index α_{eff} is the constant of the approximate separation of variables in the disk plane and in the normal direction [4]. It is determined from the solution to the 1-D problem for the natural waves propagating on a thin dielectric layer of thickness d. As a result, in the 2-D problem for the field in the median plane of the disk the bulk refractive index α has to be substituted with the effective index α_{eff} (Fig. 2 (a)). Therefore, α_{eff} depends on frequency, as well as the number and type of the natural wave of dielectric layer if its thickness is not small.

The lasing eigenvalue problem for the 2D model of uniformly active thin disk has been considered in [8,9]. It assumes that the field satisfies 2D Helmholtz equation with a complex refractive index $\nu = \alpha_{eff}^{H,E} - i\gamma$ inside the circle $r < a$ and $\nu = 1$ if $r > a$. At the circle boundary the field tangential component must be continuous. Besides, the fields must satisfy the condition of local energy finiteness and 2D radiation condition of Sommerfield at $r \to \infty$. In the analysis of active dielectric resonators we look for the modified eigenvalues, which are the pairs of positive numbers $\kappa = ka$ and γ . The first of them is the normalized lasing frequency and the second is the threshold value of material gain.



(a) (b)

Fig. 2. (a) Thin 3D dielectric resonator and corresponding structures of reduced dimensionalities. (b) Near field of the dipole type supermode of the maximum anti-symmetry in the cyclic photonic molecule of 10 active disks.

Implementation of the method of separation of variables enables one to establish that all the modes in a circular dielectric resonator split into independent orthogonal families with respect to the azimuth index $m = 0,1,2,\ldots$ and are twice degenerate if $m > 0$. For the modes of each family, transcendental equations are derived whose roots generate discrete values of κ and γ. Asymptotic analysis of these equations [9] shows that the lower modes whose family index $m \ll \kappa_{mn}^{H,E}$ have large radiation losses, and their thresholds are

$$\gamma_{mn}^{H,E} \approx \ln[(\alpha+1)/(\alpha-1)](\pi / 2\kappa_{mn}^{H,E}) \tag{1}$$

If the opposite is true, i.e. $m \gg \kappa_{mn}^{H,E} \gg m/\alpha$, then the corresponding modes are the whispering gallery modes whose thresholds decrease exponentially with frequency or index *m*,

$$\gamma_{mn}^{H,E} \approx const\ e^{-2m\ln(2m/\kappa_{mn}^{H,E})} \tag{2}$$

Here, the asymptotic expression for the normalized frequency of lasing is as follows

$$\kappa_{mn}^{H,E} \approx (\pi / 2\alpha)(m + 2n \mp 1/2)\ , \tag{3}$$

where *n* is the radial mode index and the signs ± correspond to the E_z and H_z -polarized modes, respectively.

IV. Photonic Molecules

The simplest structure of this type is a pair of identical active circular resonators considered in [10]. This is a 2-D model of the pair of thin disks located in the same plane. Such geometry has two lines of symmetry and therefore its supermodes split into four orthogonal classes with different symmetry properties relatively to these lines. For each class supermodes, the use of partial separation of variables, together with boundary conditions and conditions of local power finiteness and radiation, leads to homogeneous infinite-matrix equations of the Fredholm second kind. Thanks to the spectral equivalency with original problem, the eigenvalues coincide with the zeroes of corresponding determinant. They can be found numerically after truncating the matrix to finite order. The convergence of approximate eigenvalues to the accurate infinite-matrix ones is guaranteed by the Fredholm nature of the matrix operator.

The computation of the lasing eigenavues for the supermodes of all four classes build on the whispering gallery modes in each disk have shown that the thresholds can be both higher and lower then the threshold of the same mode in stand alone disk depending on the distance between the disks.

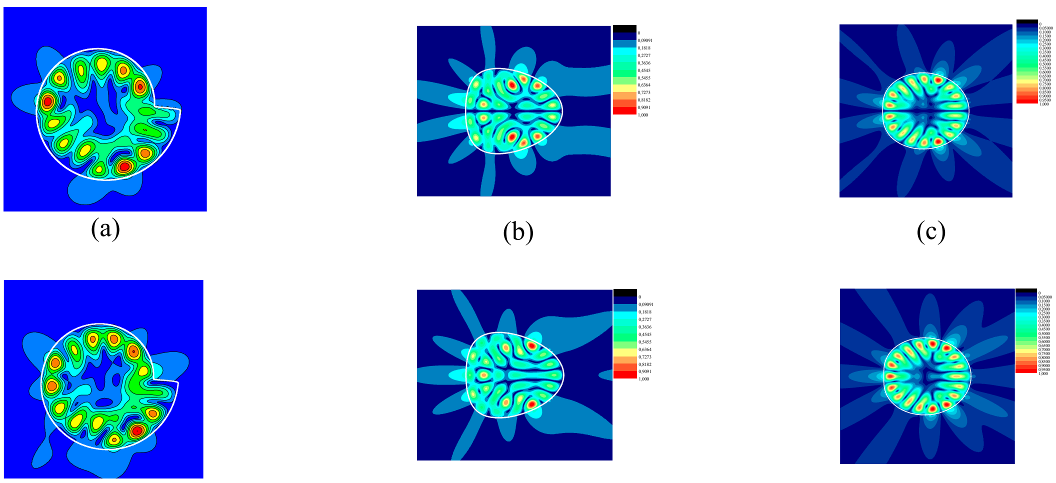
These studies have been extended to the more complicated coupled dielectric resonators shaped as cyclic photonic molecules of *M* active identical disks (Fig. 2 (b)) [11,12]. In this configuration, the number of supermode classes having different symmetry equals to *M*+1 or *M*+2 depending on the parity of *M*. Here, the most interesting are the supermodes that possess maximum degree of symmetry or anti-symmetry. For each symmetry class the lasing eigenvalue problem has been reduced to homogeneous infinite-matrix equation of the Fredholm second kind. Numerical investigation has demonstrated that the threshold can be significantly lowered by tuning the distance between elementary resonators to optimal value.

We have found a considerable difference between the properties of supermodes built on the lower (monopole and dipole) modes [12] and on the whispering gallery modes [11]. In the first case the lowering of threshold by collecting small disks in a cyclic photonic molecule takes place only for the supermodes of the maximally anti-symmetric class. This effect has non-resonant nature and is stronger for the smaller rim-to-rim distances. Besides, adding new pair of disks to photonic molecule lowers the threshold of such supermodes approximately by an order of magnitude. This is explained by a more complete canceling of partial fields radiated by adjacent disks in anti-phase to each other.

In the second case, the threshold of a whispering gallery mode of any symmetry class is low from the beginning because elementary disks are quite large. It has been found that the threshold can be lowered further, if one tunes the rim-to-rim distance properly. This effect is observed if the rim-to-rim distance is comparable to disk radius. It has resonant character: for instance, the accuracy of tuning should be of the order 1/10 of the disk radius for the modes with azimuth index $m = 5$. This is explained by a more complicated interference of the partial fields radiated by the disks of optically large dimensions.

V. Non-circular Cavities

Further we consider the set of Muller boundary IEs in the analysis of electromagnetic field in a 2-D homogeneous dielectric resonator with arbitrary smooth contour and their discretization with efficient numerical algorithm. This algorithm is further applied to the analysis of lasing frequencies and thresholds and the fields of natural H_z-polarized modes in active non-circular dielectric resonators: spiral, kite, and limacon (Fig.3).



(a) (b) (c)

(d) (e) (f)

Fig. 3. (a), (d) Near and far fields $|H_z|$ for the whispering-gallery modes of the doublet $H^{l,h}_{7,1}$ in a spiral resonator. (b), (e) Near- and far-field patterns of $|H_z|$ for the doublet of quasi-$H_{9,1}$ modes anti-symmetric (b) and symmetric (e) classes in a kite cavity. (c), (f) Near- and far-field patterns of $|H_z|$ for the doublet of quasi-$H_{9,1}$ modes anti-symmetric (c) and symmetric (f) classes in a limacon cavity.

Thin flat microcavity lasers with these resonators are attractive as configurations where a reasonable compromise can be reached between more directive light emission and reasonably low threshold of lasing.

The eigenvalue problem for the Maxwell equations with additional conditions is equivalently reduced to two coupled boundary integral equations of Muller [13] using the Green's formula. Discretization of these IEs is done by the method of qudratures (Nystrom method) [14]. This method is based on the approximation of integrals with finite sums using the corresponding quadrature formulas, which taken in account the properties of the integrand functions including their singularities. Some of the kernels of obtained equations have logarithmic singularities that should be separated. Further, we use a quadrature formula with equidistant nodes for the numerical integration of the logarithmic parts of involved integrals. Here, the integrand function is approximated by a trigonometric polynomial. The remaining smooth parts are integrated using the trapezoidal rule [15,16].

VI. CONCLUSIONS

In this paper, we have presented and discussed recently developed approach to the study of the effect of lasing using linear electromagnetic boundary-value problems. It is able to characterize not only the frequencies but also the thresholds of lasing for the natural electromagnetic fields in dielectric resonators with active regions. Within this approach, modified eigenvalue problems for several important types of 2-D dielectric open resonators have been considered. This involves stand-alone uniformly and non-uniformly active circular resonators, coupled circular resonators, and active non-circular resonators.

The results obtained enable us to consider the shape and location of the active region as engineering parameters, which can be used to manipulate with the lasing thresholds of the modes in dielectric resonators. They also show the ways for the lowering of threshold and the improvement of directionality by changing the shape of the contour (for stand-alone resonators) and by using the symmetry (for coupled resonators). Therefore they can be applied for the interpretation of the experimental data and for the design of the most promising configurations using preliminary computer-aided simulation of microlasers.

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