ESF-POLATOM Exchange Visit Grant

Accurate simulation of organic microcavity lasers shaped as flat polygons

Grant recipient: Illia Sukharevskyi

Application ref. number: 5005

Purpose of the visit

Our study was devoted to finding the eigenfrequencies of triangular resonators investigated in a recent work of our French collaborators experimentally.

Description of the work carried out during the visit

The method for the numerical analysis of the studied structures was developed, the computer code was written and verified, and the preliminary data on the spectra of triangular dielectric resonators was obtained.

Description of the main results obtained

The numerical algorithm

Consider a two-dimensional dielectric resonator D_i with complex relative permittivity or dielectric function $\varepsilon(\lambda)$ and cross-section contour L. The host medium D_e is free space. The time factor $e^{-i\omega t}$ is assumed and suppressed.

Mathematically, the electromagnetic-field eigenvalue problem can be reduced to the Muller boundary integral equations (MBIE)

$$U(\vec{r}) + \int_L K_{11}(\vec{r},\vec{r}\,')U(\vec{r}\,')ds' - \int_L K_{12}(\vec{r},\vec{r}\,')V(\vec{r}\,')ds' = 0, \quad (1)$$

$$\frac{1+p}{2}V(\vec{r}) + \int_L K_{21}(\vec{r},\vec{r}\,')U(\vec{r}\,')ds' - \int_L K_{22}(\vec{r},\vec{r}\,')V(\vec{r}\,')ds' = 0, \ \ \vec{r} \in L, \quad (2)$$

where $\vec{r} = (x, y)$ and $\vec{r}\,' = (x', y')$ are the integration and observation points, respectively; U corresponds to the field components E_z or H_z depending on polarization, in the domain D_i. Furthermore, $V(\vec{r}) = \partial U(\vec{r}) / \partial n$ is the limit value of the normal derivative of the total field on the closed contour L of the scatterer from the inner side of it, the normal unit vector $\vec{n}$ is directed to the outer domain D_e, $d\vec{r}\,'$ is the elementary arc length, and the constant is $p = 1$ in the E-polarization case and $p = 1/\varepsilon$ in the H-polarization case.

The kernels of the MBIE have the following form:

$$K_{11} = \frac{\partial G_i}{\partial n'} - \frac{\partial G_e}{\partial n'}, \quad K_{12} = G_i - pG_e, \quad (3)$$

$$K_{21} = \frac{\partial^2 G_i}{\partial n\,\partial n'} - \frac{\partial^2 G_e}{\partial n\,\partial n'}, \quad K_{22} = \frac{\partial G_i}{\partial n} - p\frac{\partial G_e}{\partial n} \quad (4)$$

where $G_{(i,e)} = G_{(i,e)}(\vec{r},\vec{r}\,') = (i/4)H_0^{(1)}(k_{i,e}\rho)$ are the Green’s functions of the corresponding homogeneous media, $k_e = k_0$, $k_i = k_0\sqrt{\varepsilon}$, and $\rho = |\vec{r} - \vec{r}\,'|$, $k_0 = \omega / c$ and c is the free-space light velocity.

For the discretization of (1), (2), we subdivide the contour L into separate smooth segments, extract logarithmic singularities from (3) and (4), and apply a quadrature rule on each segment. The discretization performed in this manner is not sensitive to the irregularities of the contour so far as the interpolation nodes do not coincide with edge points. After analyzing the kernels at $\vec{r} \to \vec{r}\,'$ and denoting the contour curvature $\varsigma(\vec{r})$, we introduce new continuous kernels as follows:

$$\tilde{K}_{11} = \begin{cases} K_{11} = \dfrac{i}{4}\left[-k_i H_1^{(1)}(k_i\rho) + k_e H_1^{(1)}(k_e\rho)\right]\dfrac{\partial\rho}{\partial n'}, & \vec{r} \neq \vec{r}\,' \\ 0, & \vec{r} = \vec{r}\,' \end{cases} \tag{5}$$

$$\tilde{K}_{12} = \begin{cases} K_{12} = \dfrac{i}{4}\left[H_0^{(1)}(k_i\rho) - pH_0^{(1)}(k_e\rho)\right], & \vec{r} \neq \vec{r}\,' \\ (1-p)\left(\dfrac{i}{4} - \dfrac{C}{2\pi}\right) - \dfrac{1}{2\pi}\left(\ln\dfrac{k_i}{2} - p\ln\dfrac{k_e}{2}\right), & \vec{r} = \vec{r}\,' \end{cases} \tag{6}$$

$$\tilde{K}_{22} = \begin{cases} K_{22} = \dfrac{i}{4}\left[pk_e H_1^{(1)}(k_e\rho) - k_i H_1^{(1)}(k_i\rho)\right]\dfrac{\partial\rho}{\partial n}, & \vec{r} \neq \vec{r}\,' \\ \dfrac{1-p}{4\pi}\varsigma(\vec{r}), & \vec{r} = \vec{r}\,' \end{cases} \tag{7}$$

$$\tilde{K}_{21} = \begin{cases} K_{21} = \dfrac{i}{8}\Big[k_e^2 H_0^{(1)}(k_e\rho) - k_i^2 H_0^{(1)}(k_i\rho) \\ +k_i^2 H_2^{(1)}(k_i\rho) - k_e^2 H_2^{(1)}(k_e\rho)\Big]\dfrac{\partial\rho}{\partial n}\dfrac{\partial\rho}{\partial n'} \\ +\dfrac{i}{4}\left[k_e H_1^{(1)}(k_e\rho) - k_i H_1^{(1)}(k_i\rho)\right]\dfrac{\partial^2\rho}{\partial n\,\partial n'}, & \vec{r} \neq \vec{r}\,' \\ \dfrac{k_i^2 - k_e^2}{4\pi}\left(\dfrac{i\pi}{2} - C\right) - \dfrac{1}{4\pi}\left(k_i^2\ln\dfrac{k_i}{2} - k_e^2\ln\dfrac{k_e}{2}\right), & \vec{r} = \vec{r}\,' \end{cases} \tag{8}$$

Introduce N sub-sections of the lengths Δ_j $(j = 1,\ldots,N)$ of the segments of L and assume that unknown functions are constants at each sub-section. Then, after applying the rectangle rule for numerical integration, we obtain the following matrix equation:

$$K\begin{pmatrix} U \\ V \end{pmatrix} = 0, \tag{9}$$

where $U = \{U(\vec{r}_i)\}_{i=1}^{N}$, $V = \{V(\vec{r}_i)\}_{i=1}^{N}$, and

$$K = \begin{pmatrix} 1 + \tilde{K}_{11}(\vec{r}_i,\vec{r}_j)\,|\Delta_j| & -\tilde{K}_{12}(\vec{r}_i,\vec{r}_j)\,|\Delta_j| - (p-1)\displaystyle\int_{\Delta_i}\ln\rho\, ds' \\ \tilde{K}_{21}(\vec{r}_i,\vec{r}_j)\,|\Delta_j| + \dfrac{k_i^2 - k_e^2}{4\pi}\displaystyle\int_{\Delta_i}\ln\rho\, ds' & \dfrac{1+p}{2} - \tilde{K}_{22}(\vec{r}_i,\vec{r}_j)\,|\Delta_j| \end{pmatrix}.$$

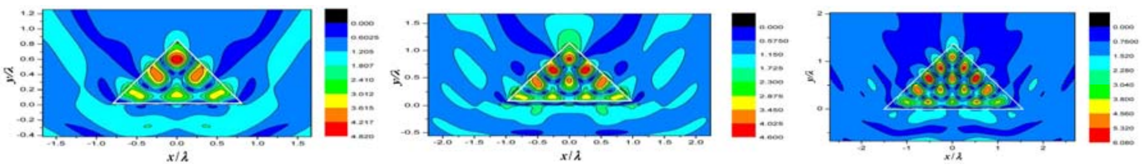
As $\rho = |\vec{r} - \vec{r}\,'|$, the value of $\int_{L_i}\ln\rho\, ds'$ can be obtained analytically.

Let a be a characteristic size of resonator (for instance, a base of triangle). Then, the eigenvalues $\chi = k_0 a$ are the roots of a determinantal equation,

$$\det K(\chi) = 0.$$

Some preliminary results

The following plots demonstrate right-angle dielectric prisms excited in the near-to-complex-resonances real frequencies by the H-polarized wave incident on the base of triangle.



(a) $k_0 a = 10.5$ (b) $k_0 a = 14$ (c) $k_0 a = 17$

<u>Future collaboration with host institution</u>
After constructing numerically the resonant fields of thin triangular cavities of polymer lasers, we will compare them with experimental patterns, in order to assign them to a certain type of complex resonance. The next step of our collaboration will be a study of the lasing spectra and thresholds of a pumped cavity.

<u>Projected publications</u>
The support of ESF network “POLATOM” was acknowledged in the following conference paper:
A.I. Nosich, E.I. Smotrova, M. Lebental, I.O. Sukharevsky, A. Altintas, Microcavity lasers on polymer materials: boundary integral equation modeling and experiments, *Proc. Int. Conf. Electronics and Nanotechnologies (ELNANO-2015)*, Kiev, Ukraine, 2015.

In coming months we are planning to publish a journal paper. The publication will acknowledge the project.