Numerical modeling of the spectral and spatial distribution of the electromagnetic modes in a tunable microcavity for investigation of the light-matter interaction.

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Abstract. The light-matter interaction between a molecule and confined electromagnetic field is of great interest because it allows tuning the energy states and the spectral properties of the coupled matter. This effect offers a great number of applications in many areas, such as nonlinear physics, biosensing and lasing. The most widely used approach to achieve light-matter coupling is to place an ensemble of molecules inside an optical cavity. In order to maximize the effects of interaction, it is necessary to model the spectral properties of the cavity in order to find the optimal parameters for the experiments. In this study, the model for the numerical calculation of the spectral and spatial properties of electromagnetic modes of a tunable microcavity was developed and a mode analysis has been performed. The cavity transmission spectra and the electromagnetic field distribution were investigated. The results showed a good agreement with the experimental data obtained earlier.

1. Introduction
The resonant interaction between a confined electromagnetic field and molecules is of fundamental importance for a wide range of scientific fields and technology. One of the possible ways to confine the electromagnetic field is to employ an optical microcavity. When the rate of coherent energy exchange (coupling strength) exceeds the total losses of the hybrid system, the strong coupling regime is being reached [1]. This regime is characterized by the formation of the new states with the energy difference being proportional to the coupling strength [2]. In order to maximize the coupling strength, it is necessary to minimize the electromagnetic mode volume of the cavity. In practice, in order to find the optimal parameters of the experiment and to properly analyze its results, it is important to model the optical properties of a cavity. Recently, in our group, tunable microcavity has been developed for the investigation of the light-matter coupling. Details on the design and implementation of the microcavity could be found elsewhere [3,4]. Briefly, the microcavity consists of unstable Fabry-Perot microresonator formed using the upper convex mirror and the lower plane metallic mirror placed on a piezoelectric actuator. To calculate the key optical parameters (Q-factor, mode volume, and field distribution) of the microcavity it is necessary to develop an appropriate mathematical model. This cavity with plane-convex mirrors have several advantages, such as high precision tunability of the resonance wavelength for coupling to...
the molecular transition which is provided by precise control of cavity length using the piezoelectric actuator and effortless sample replacement. The convex shape of the mirror ensures the confinement in transverse direction. Here, the numerical method of modeling should be used, as an exact analytical solution for this geometry seems to be impossible due to the convexity of one mirror and subsequent inapplicability of analytical methods developed for resolution of one-dimensional problems.

In the present study we propose a numerical approach for modeling the optical properties of the microcavity. We show that by accurately selecting the conditions and by taking into account the exact geometry of the microcavity, good agreement between the stimulated and experimental data can be reached. The modeled data allow very correctly estimate the key optical parameters of the microcavity modes.

2. Method
Our model relies on the finite elements method [5], which is based on the fragmentation of the calculating area, numerically solving the Maxwell’s equations for each cell separately and connecting solutions in adjacent fragments. An important advantage of this method is simplicity of taking into account the material properties such as the refractive index and extinction coefficient.

The wavelength dependences of the refractive index and the extinction coefficient for silver films which were used as mirrors of our microcavity were taken into account using the data given in [6]. The space between the mirrors was filled with immersion oil. In our model we considered that the medium has no losses and its refractive index is constant and equal to 1.51.

3. Results and discussion
Firstly, the dependence of the electromagnetic field energy inside the microcavity on the wavelength of the electromagnetic wave was investigated. For the cavity length of $2.12 \, \mu m$, the calculated spectrum was compared with the experimental transmission spectrum, that had been measured previously (Figure 1).

![Figure 1](image-url)

**Figure 1.** The calculated spectral distribution of electromagnetic field energy inside the microcavity (black), and the experimental microcavity transmission spectrum (red).

It can be seen that modeled spectrum adequately describes the positions of the transmission maxima which correspond to the longitudinal modes of the microcavity. However, in other spectral regions the modeled spectrum does not coincide with the experimental one. In particular, we can see that calculated peaks are wider and have an asymmetric shape. This fact is caused by the superposition of the accessory peaks corresponding to the higher transverse modes. Small difference in eigenenergies
of these transverse modes leads to the merging into continuous high energy wing near each longitudinal mode. For better agreement between the modeled and experimental spectra we took into account the square size of the measurement area of the experimental system in a confocal regime. The comparison of the corresponding calculated and experimental spectra is presented on figure 2.

![Figure 2](image)

*Figure 2.* The calculated spectral distribution of the electromagnetic field energy inside the microcavity taking into account the confocal regime (black), and the experimental microcavity transmission spectrum (red).

As one can see reducing the area in transverse direction down to 400 nm for calculation the transmission spectrum allows to eliminate the accessory peaks in the modeled spectrum. Thus, decrease of calculating area made possible the mode selection by ignoring the higher transverse modes. After this correction (or procedure) the calculated spectrum agrees well with the experimental one. In particular, the positions and the widths of the modeled peaks coincide with the data that had been measured previously. This fact proves that the developed model correctly calculates the parameters of tunable microcavity such as the Q-factor which was estimated to be 110 for the central mode on the graph. Also, for the central peak of the spectra, the spatial distribution of electromagnetic energy inside the cavity was computed (Figure 3).

![Figure 3](image)

*Figure 3.* The spatial distribution of the electric field inside the cavity for the eigenmode with the resonant wavelength of 570 nm. The top and bottom edges of the figure correspond to the convex and plane mirrors, respectively. The vertical black solid lines limit the area used for the calculation of the transmission spectrum (the distance between them is equal to 400 nm). The horizontal image size characterizes the effective area of field localization, which is equal to 7 μm.
The figure shows that for the eigenmode with resonant wavelength of 570 nm the electromagnetic field inside the cavity is relatively highly confined. For the numerical evaluation of this confinement area the mode volume was calculated using the following formula:

$$V_m = \frac{\int_V |E|^2 dV}{|E_{\text{max}}|^2},$$

where \(E\) is the electric field strength and \(E_{\text{max}}\) is the maximum of the electric field strength inside the cavity. The mode volume was estimated to be 70 in units of \((\lambda/n)^3\). For comparison, the typical values of the effective modal volume in optical microcavities are \(\sim 10^5\) [2]. Due to the inverse square root dependence of the coupling strength on the mode volume, such a decrease in the value of \(V_m\) can lead to an increase in the coupling strength by more than an order of magnitude.

### 4. Conclusion

In this study, the model for the numerical calculations of the spectral properties of a tunable microcavity was developed and the mode analysis was performed. The cavity transmission spectra and the electromagnetic field distribution were investigated. The results showed a good agreement with the experimental data obtained earlier. Importantly, the calculated value of the mode volume of the eigenmode with a resonant wavelength of 570 nm has been found to be at least three orders of magnitude smaller than that of the typical planar Fabry-Perot microcavities, which are widely used for the investigation of the light-matter interactions.

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