Numerical analysis of subwavelength field effects in photonic crystal slab cavities

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Abstract
Surface coupling of single quantum emitters to optical cavities consisting of a photonic crystal slab is a delicate yet crucial task for photonic quantum applications. By coupling through the evanescent surface field only small Purcell factors can be achieved. Here, we propose to introduce a pit in the slab to position the emitter closer to the mode field maximum. Photonic crystal slab L3 cavities are investigated with respect to quality factor and Purcell effect, using finite element calculations in the frequency domain. That way the spatial distribution of the Purcell factor can be calculated. Introducing a small sized pit to the surface of the photonic crystal cavity can evoke subwavelength field effects, confining the field maximum inside the pit. By engineering a pit in the center of the cavity the Purcell factor can be increased from 176 to 1331, albeit reducing the Q factor from 20769 to 16696.

1. Introduction

Photonic crystal (PhC) cavities pose a promising platform for quantum information technology or nanoscale sensors [1–3]. These cavities exhibit low losses, strong spatial light confinement to volumes smaller than the cubic wavelength as well as high Q factors, thereby enabling strong interaction with quantum emitters such as atoms, molecules or quantum dots [1]. They allow for strong emitter-cavity coupling in single photon sources for quantum information processing, quantum computing or bio-sensing [4–6]. High Q factors and small mode volumes lead to a strong Purcell effect \( P_P \sim Q/V_{gh} \), which states that the rate of spontaneous emission can be controlled by the dielectric environment via the local density of photonic states. To further decrease the effective mode volume to subwavelength dimensions high dielectric contrast discontinuities can be employed, enhancing the electric field in the low index material. This can be done by slots [7] or dielectric nanoantennas [8]. This mechanism is used for cavities as well as for waveguides [7–11], but also applies for evanescent fields at total internal reflection [12].

Cavities composed of two-dimensional photonic crystals possess in-plane confinement by periodic holes, with a central defect as cavity, and vertical confinement by a semiconductor slab. A typical defect is the L3 cavity, where a line of three holes are missing. By minor additional refinements in the design, the Q factor can be increased significantly. They consist of shifting and reducing radii of near cavity holes, as shown for L3 cavities [13–16], H0 cavities [15, 17] and L3 cavities surrounded by different media [18, 19].

However, determining the Purcell factor via the ratio of Q factor and mode volume is only an approximation [12]. Furthermore the Q factor accounted in this approach is an effective Q factor, determined by the cavity and emitter, limiting the impact of the cavity’s Q factor [7, 20]. In the direct approach the density of states can be calculated via the Green’s function.

An attractive configuration for a quantum light source places the emitter at the surface of the photonic crystal slab, which is convenient for fluorescent molecules. Alternatively, semiconductor emitters such as quantum dots can be fabricated inside the slab material. For quantum emitters placed at the surface it is crucial to achieve sufficient electromagnetic coupling to the cavity. Different approaches have been reported so far, such as placing the emitter on the slab surface in the center of the cavity or inside an adjacent hole [21, 22].

We propose and investigate the possibility of making a nano-pit on the slab surface in the center of the cavity to facilitate both the deterministic emitter placement and its coupling to the cavity mode. Similar approaches

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have been reported for sensor systems, but without analyzing the electric field intensity distribution and Purcell factor [3].

The photonic crystal cavity is investigated using 3D finite element (FE) simulation, which solves Maxwell’s equations. From the resulting electric fields it is possible to directly calculate the Purcell factor and investigate its spatial distribution [23]. That way we can determine the best placement of the emitter to achieve strong coupling and investigate the impact of features added to the crystal, such as a pit, on the Purcell factor.

In section 2 the setup of the model and the methods used here are described. The results are presented in section 3.

2. Methods

The analysis of the photonic crystal cavity is performed using a 3D FE Maxwell solver, developed in our group [23, 24]. It solves the wave equation in frequency domain (equation (1)).

\[ \nabla \times \varepsilon^{-1} \nabla \times \vec{E} - k^2 \varepsilon \vec{E} = -jkZ_0 \vec{j} , \]

where \( \vec{E} \) is the electric Field, \( \vec{j} \) is the source current density, \( Z_0 \) is the vacuum wave impedance, \( k \) is the wavenumber, \( \varepsilon \) and \( \mu \) are tensors for the permeability and permittivity, respectively. Setting the right hand side inside the cavity, with \( k_R \) consists of a pitch \( a \) of 240 nm, a hole diameter \( d \) of 170 nm and a slab thickness \( t \) of 150 nm results in a resonance around 800 nm for the fundamental mode (figure 2). These values were obtained by first calculating the photonic band structure for an infinite photonic crystal slab using the open source code MIT photonic bands (MPB) and subsequent FE simulations for a finite L3 cavity, as described above [27]. The fundamental mode consists of an \( x \)- (figure 2(b)) and \( y \)-polarized (figure 2(c)) field component, where the \( x \)-polarized part covers the center of the cavity and the \( y \)-polarization portion is near adjacent holes. The schematics of the lattice are shown in figure 3. A Q factor of about 3500 is obtained for a L3 cavity with no further modifications. On the slab surface a maximum Purcell factor of 110 can be achieved, at the location of the intensity maximum. Nevertheless, a Purcell factor of 246 is calculated inside a PhC hole adjacent to the cavity as schematically indicated in figure 3. These values are valid for perfect alignment of the polarization of the emitter and the mode field. That corresponds to \( y \)-polarization in an adjacent hole (figure 2(c)) and \( x \)-polarization for center placement (figure 2(b)).

An effective method to achieve high Q factors in PhC cavities is to shift the innermost holes to the cavity outwards [13]. In our case, with a shift of the two innermost holes to the cavity by 0.18a (see figure 3), the Q
factor is increased to 20796, as extracted from the complex eigenvalue. This value is comparable, though slightly higher, to other values reported for L3 GaP cavities [21, 28]. There, a $Q$ factor above 10000 in finite difference time domain (FDTD) simulations and up to 1700 in experiments was reported for a target wavelength of 645 nm with following parameters: pitch $a = 255$ nm, hole diameter $d = 153$ nm, slab thickness $t = 140$ nm and an outward shift of the next to cavity holes by $0.15a$ [28]. The $Q$ factor is dependent on the lateral extension or number of periods of the photonic crystal. The model used here provides a finite size, just as a fabricated photonic crystal.

The Purcell factor for this case is increased to 176 for an emitter on the slab surface (center of mode placement), and to 567 inside an adjacent hole (figure 3). If the emitter is placed inside the slab layer, at the center of the cavity, a Purcell factor of up to 874 can be obtained.

In order to maximize the coupling for a surface emitter to the electromagnetic PhC mode, a cylindrical pit is introduced in the upper surface of the slab. This has been shown to reduce the effective mode volume in dielectric cavities [7]. The pit is located where the maximum of the $E_z$ component of the mode is expected. The positions of emitter placement are illustrated in figure 4.
Optimizing the depth and diameter of the pit a Purcell factor of 1331 can be achieved for a depth of 50 nm and a diameter of 17 nm, as can be seen in figure 5. This is a significant improvement compared to an emitter placement on the flat surface of the cavity. The Q factor of the cavity drops to 16700 when adding the pit, and the resonance wavelength is marginally influenced. The results are summed up in table 1. In the following, the optimization process for choosing the pit dimensions is described in more detail. Figure 6 shows the dependence of the Q factor on the pit diameter (at fixed depth of 50 nm). Only diameters smaller than 50 nm show a strong coupling of the emitter to the cavity, with a Purcell factor of up to 1331, translating to an effective mode volume of $0.9533\left(\frac{\lambda}{n}\right)^3$. The depth of the pit has less influence on the Q factor, but a trend for the Purcell effect becomes apparent, as shown in figure 7. The deeper the pit, the higher the Purcell factor, corresponding to a lower mode volume (from $8.94\left(\frac{\lambda}{n}\right)^3$ for no pit to $0.53\left(\frac{\lambda}{n}\right)^3$ for the deepest pit). For the subsequent discussion, we choose the case of 50 nm pit depth, which allows a realistic aspect ratio with respect to the diameters discussed before.

In general, the increase of the Purcell factor in the pit is due to a field enhancement effect that appears at high discontinuities for the refractive index. At a boundary between two materials, the normal component of the dielectric displacement $D_{\text{norm}}$ needs to be continuous. Therefore a high discontinuity in the refractive index results in a high electric field difference, with the stronger field in the low index material. This explanation can be
verified by analyzing the fields in the PhC cavity and the pit. Within the cavity center the field of the respective mode is \(x\)-polarized, such that it constitutes the normal component for the interface to the pit along the \(x\)-axis (see figure 2). This field enhancement effect however, is dependent on the size of the pit, where the diameter is more influential than the depth, as already discussed (figures 6 and 7). Figure 8 compares the field intensity distribution for a slab without a pit to a pit of fixed depth (25 nm) and different diameter (170 nm and 21.25 nm). For the large pit diameter the peak value of the field intensity distribution is lowered. Nevertheless, it can be seen that, as the diameter of the pit decreases the field enhancement at the boundary increases, finally resulting in a high field distribution throughout the whole pit. The polarization of the field is homogeneous.
throughout the pit and identical with the polarization of the cavity mode. The field vectors within the pit are shown in figure 2(d). Knowledge about the polarization of the mode and placement of the emitter is crucial, as the emitter polarization should be the same as the mode to achieve the highest coupling and Purcell effect.

To determine whether the coupled system will be in the strong or weak coupling regime knowledge or assumptions about the emitter need to be provided. The condition for strong coupling is:

$$16g^2 > (2\kappa - \gamma)^2,$$

where $g$ is the coupling constant and $\kappa$ and $\gamma$ are the decay rates of the cavity and the emitter, respectively [25]. This condition is stronger than others found in literature, resulting in smaller lifetimes required for achieving the strong coupling regime [4]. The coupling constant as well as the emitter decay rate depend on the radiative lifetime ($T$) of the emitter, with:

![Figure 7. Q and Purcell factor in dependence of depth of pit with a fixed diameter of 17 nm.](image7)

![Figure 8. Field intensity in the center of the cavity for pits with fixed depth (25 nm) and different diameter. As the diameter decreases the field localization and enhancement increases.](image8)
where $F_p$ is the Purcell factor. Both sides of the condition (in equation (4)) depend on the lifetime of the emitter.

In order to determine whether the strong coupling regime is achieved for a given emitter, both sides of the condition with respect to emitter lifetime are shown in Figure 9, using the values obtained before (see Table 1 for the case with pit). From the plot it can be derived that an emitter with a lifetime less than about 37.5 ns would be in the strong coupling regime. Semiconductor quantum dots, with a lifetime of about 1 ns or 1.5 ns would be in the strong coupling regime [4, 25], as well as molecules, such as DBATT, with lifetimes around 10 ns [29]. Introducing the impact of imperfections in the fabrication process or additional material losses, resulting in lowered $Q$ and Purcell factor by a factor of 10 will shift the critical lifetime from 37.5 ns to about 0.4 ns.

We assume that fabricating such small features will be challenging but not unrealistic. For example, fabrication of features such as slots or holes in photonic crystals with dimensions less than 40 nm and very high aspect ratios (50:1 compared to around 3:1 here) were reported in [3, 10, 30].

4. Conclusion

We have presented a numerical analysis of Purcell effect and subwavelength field effects in photonic crystal slab cavities. The goal was to couple an emitter, such as a molecule, located on the surface of the slab to the electromagnetic cavity mode. By introducing a nano pit to the slab surface it is possible to enhance the Purcell effect for the emitter substantially, albeit reducing the $Q$ factor. The root cause of this improvement is due to subwavelength field enhancement, which results from high refractive index discontinuities. By numerical analysis of the field intensity for the example of a GaP L3 cavity at 800 nm, this assumption could be confirmed.

An optimized L3 cavity exhibits a $Q$ factor of 20800, and an electromagnetic emitter placed directly on the slab surface exhibits a Purcell factor of 176. In contrast, placing the emitter in a nano pit on the surface with a diameter of 17 nm and a depth of 50 nm, a Purcell factor of 1331 can be obtained. This is an increase by a factor of 7.5 compared to the placement on the unmodified surface. With the nano pit configuration, emitters with short radiative lifetimes such as quantum dots are well in the strong coupling regime.

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