Optimization of circular photonic crystal cavities – beyond coupled mode theory

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Abstract: We study comprehensively using numerical simulations a new class of resonators, based on a circular photonic crystal reflector. The dependence of the resonator characteristics on the reflector design and parameters is studied in detail. The numerical results are compared to analytic results based on coupled mode theory. High quality factors and small modal volumes are found for a wide variety of design parameters.

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References and links

1. Introduction

Circular optical resonators are becoming key components in modern optical communication systems and devices. Numerous applications for optical communications have been demonstrated such as filters [1], add/drop multiplexers [2, 3], delay lines [4-6] and modulators [7] as well as for sensing [8], spectroscopy and basic research in quantum electrodynamics (QED), nonlinear optics and similar fields [9, 10].

For many of these applications, it is desirable for the resonators to exhibit both compact dimensions and high quality factor (Q), which is a measure of the power dissipation rate from the cavity. These requirements are mutually contradictory for conventional resonators utilizing the total internal reflection (TIR) mechanism to confine the light. While for cavity radii much larger than the wavelength, high Q can be achieved, as the radius is reduced, the effectiveness of the TIR mechanism decreases, introducing loss which consequently reduces the Q of the cavity. This loss mechanism is often addressed as “bending losses”.

This link between the bending losses and the cavity dimensions can be broken in resonators employing distributed Bragg reflection instead of TIR. Such resonators, e.g., Photonic Crystal (PC) defect cavities [11-16] and Circular Bragg resonators [17-21] have been suggested and studied before, demonstrating ultra-small modal volume and high Q although not as high as demonstrated in other types of cavities. Consequently, significant efforts were devoted to improving the Q of PC cavities. Generally speaking, the cavity Q can be separated into two contributions – the in-plane or horizontal Q (Q∥) and the out-of-plane or vertical Q (Q⊥) associated with the power radiating from resonator in the slab plane and perpendicular to the slab plane respectively. While the in-plane losses (determining Q∥) can be, in principle, arbitrarily reduced by increasing the length of the reflector (the number of Bragg layers), the out-of-plane losses are more complicated to minimize. It has been shown, that the out-of-plane Q can be improved by rearranging the positions and dimensions of the holes of the PC reflector to reduce the intensity of the field components lying within the light cone [22, 23]. The idea underlying the optimization process is to “soften” the edge of the cavity in order to construct a more “smooth” field profile [15]. Nevertheless, such optimization requires a tedious procedure of tailoring the position and size of each hole in the PC reflector.

Recently, it was suggested to employ radial Bragg layers instead of PC to confine light in small cavities [24]. The radial structure offers significant advantages for optimal cavity design, primarily because it enables analytic design of the layer structure and optimal tailoring of the cavity size and the reflector periodicity. Unfortunately, the radial Bragg structure is
difficult to realize using the suspended membrane concept which was successfully used for PC cavities. In addition, the upper surface of such structure is not continuous which makes it less suitable for electrical pumping and for realizing electrically pumped micro-lasers. To facilitate that, a new type of circular resonator based on PC reflectors was proposed [17, 18] (see Fig. 1). The generic structure consists of a solid disk surrounded by a perforated area of holes which serves as a distributed feedback reflector (DBR). Such structure can be realized using the suspended membrane concept and to be electrically pumped while retaining the advantages of the circular geometry.

![Three images showing different lattice structures](1a) (1b) (1c)

Fig. 1. Circular PC reflector structure. (a) rectangular lattice (b) triangular lattice (c) sunflower lattice

In this paper, we use three-dimensional Finite Difference Time Domain (FDTD) simulations to comprehensively study circular PC resonator structures. The generic structure is shown in Fig. 1. The arrangement of the holes defines the type of the reflector. Specifically, we focus on three different types of structures: the rectangular lattice (Fig. 1a), the triangular lattice (1b) and the “sunflower” lattice (1c). The rectangular lattice structure is a cylindrical counterpart of the rectangular PC in Cartesian coordinates. Each “necklace” consists of identical number of holes and the angular length of the holes increases for larger radii. The holes in the triangular lattice structure are arranged in a similar way but with a half period shift in the azimuthal direction. The sunflower lattice structure comprises holes of the same angular size where the number of holes in each concentric ring is proportional to the circumference of the ring.

In section 2, we briefly discuss the design of our structures, in section 3 we present the studied structure and the results obtained from the FDTD simulations, and in section 4 we discuss the results and summarize.

2. Structural design

We consider a resonator structure of the type shown in Fig. 1. These structures consist of two regions: 1) A solid dielectric disk and 2) A perforated area which serves as a distributed feedback reflector. Because of the cylindrical geometry, the TM modal field solution in the central disk is a superposition of the Hankel functions of the first and second kind [25]:

\[
H'_z(x) = A \cdot H^{(1)}_m(x) + B \cdot H^{(2)}_m(x)
\]  

where \(H_z\) is the z component of the magnetic field, \(H^{(1,2)}_m\) are respectively the \(m^{th}\) order Hankel functions of the first and second kind, \(x = k_0\eta_{eff}\rho\) is the normalized radius, \(k_0\) is the wavenumber in vacuum, \(\rho\) is the radial coordinate, and \(\eta_{eff}\) is the effective index of the slab in the vertical dimension (this parameter is used in order to reduce the 3D problem to an effective 2D one). In the spirit of coupled mode theory (CMT), the field profile in the perturbed region can be represented in a similar fashion where the amplitudes \(A\) and \(B\) vary slowly in \(x\):

\[
H'_z(x) = A(x) \cdot H^{(1)}_m(x) + B(x) \cdot H^{(2)}_m(x)
\]  

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Following conventional derivation of CMT, it can be shown that the required dielectric profile for efficiently coupling between the outgoing ($H^{(1)}$) and incoming ($H^{(2)}$) waves is given by [19]:

$$
\varepsilon(x, \theta) = \begin{cases} 
  n_0^2 - (n_0^2 - n_p^2)\Im\{2\phi(H_m^{(1)}(x)), \alpha_r\} \Im\{l\theta, \alpha_\theta\}, & x > x_0 \\
  n_0^2, & x \leq x_0 
\end{cases} \tag{3a}
$$

$$
\Im(y, \alpha) = \begin{cases} 
  0, & \sin(y) < \alpha \\
  1, & \sin(y) \geq \alpha 
\end{cases} \tag{3b}
$$

where $x_0$ indicates the (normalized) radius of the inner disk, $-1 < \alpha_r < 1$, $-1 < \alpha_\theta < 1$, $l$ is the angular (spatial) frequency of the perturbation, $\phi$ indicates the phase function and $n_0$ and $n_p$ are respectively the material and “holes” indices of refraction. The parameters $\alpha_r$ and $\alpha_\theta$ represent threshold levels that determine the angular and radial size of the holes in the reflector region where larger $\alpha$’s indicate smaller holes and, correspondingly, weaker perturbation.

The index structure (3) generates a circular cavity with a rectangular photonic crystal reflector (Fig. 1(a)). The triangular and sunflower reflectors shown, respectively, in Figs. 1(b) and 1(c) can be constructed in a similar way by slightly modifying (3). In the triangular lattice, every second “necklace” of holes is rotated by a half of a cycle compared to the rectangular lattice and in the sunflower lattice, the number of holes in each “necklace” is increased linearly with the radius in order to retain the angular size of the holes. Other lattice configurations can be envisioned as well, e.g. lattices with random rotation of each “necklace” of holes, lattices with circular holes, etc. but the study of such configurations is beyond the scope of this paper. Nonetheless, it is important to note that from the CMT point of view, the angular dependence of the perturbation is of less significance and that it is the radial part of the perturbation which determines the modal field profile [18].

For the index profile (3), the radial mode profile consists of a Bessel function in the central disk and an exponentially decaying Bessel function in the reflector region [18]. The decay constant depends on the strength of the perturbation which is affected by the threshold levels $\alpha_r$ and $\alpha_\theta$:

$$
H_r(x) = \begin{cases} 
  J_m(x), & x < x_0 \\
  J_m(x)\exp[-k(x-x_0)], & x \geq x_0 
\end{cases} \tag{4}
$$

where $k$ is the coupling coefficient between the radially incoming and outgoing waves, given by $k = \Delta \varepsilon_0 / m_0^2$ and $\Delta \varepsilon_0$ is the DC component of the Fourier expansion of the reflector index profile. For the “rectangular” lattice (3), this component is given by:

$$
\Delta \varepsilon_0 = -2 \cdot (n_0^2 - n_p^2) \cos[\sin^{-1}(\alpha_r)] \cdot \cos^{-1}(\alpha_\theta) / \pi^2 \tag{5}
$$

Equation (5) illustrates the impact of the various parameters on the coupling coefficient and, correspondingly, on the radial mode profile (4). As can be expected, decreasing $\alpha_r$ and $\alpha_\theta$ results in a stronger coupling coefficient and a more confined mode profile. Although (3a) represents the index profile of the “rectangular” reflector, it can be straightforwardly shown that the coupling coefficients of the “triangular” and “sunflower” reflectors are identical (for the same values of $\alpha$ and $\alpha_\theta$—see [19] for more details).

3. Simulation results

In our simulations, we consider a 0.3 $\mu$m thick dielectric slab with refractive index of 3.4 suspended in air. For the TM ($H_z$) polarization, this configuration yields a vertical effective index of 2.86 at the design wavelength of 1.55$\mu$m. The radius of the inner disk is 1 $\mu$m and the reflector covers the rest of the horizontal computation area. We designed the dimensions
of our structure for the 8th angular mode \((m=8)\). The computation volume is 10.6 \(\mu m \times 10.6 \mu m \times 2.1 \mu m\). The spatial and temporal resolutions of our simulations are respectively 26.5 nm and 0.08 fs. The simulation time interval is approximately 60 ps. The structure is excited with a short, broad-band, pulse (~2ps), and second order Mur absorbing boundary conditions [26] are employed to reduce the influence of reflections from the computation boundaries.

We are primarily interested in four different aspects of the resonator structure and how they affect the \(Q\), the resonance wavelength and the modal volume. The quality factor is evaluated according to \(Q = \omega_0 \tau_0\) where \(\omega_0\) is the resonant frequency and \(\tau_0\) is the cavity ring-down time constant. Both quantities \((\omega_0\) and \(\tau_0)\) are directly extracted from the FDTD simulation. Among the three lattice types presented above, we focus on the sunflower reflector because both 2D and 3D simulations predict superior \(Q\) for this type of lattice [19].

![Field Profile of high Q and low Q for a “sunflower” resonator with \(l=70\), \(\alpha_r=0\) and \(\alpha_\theta=0.1\)](image)

Figure 2 depicts a cross-section of the z component of the magnetic field \((H_z)\) at the center of the slab at \(t = 60ps\). It illustrates the difference between a field profile with high \(Q\) and one with low \(Q\) for a “sunflower” structure with \(l=70\), \(\alpha_r=0\) and \(\alpha_\theta=0.1\). In Fig. 2a, the high \(Q\) field is symmetric and well confined to the center of the disk. The low \(Q\) field shown in Fig. 2b exhibits distortion due to beating between two close resonance frequencies, but more importantly, the field is not well confined and therefore exhibits more loss.

![Comparison between theoretical (red) and numerical (green) radial field profile](image)

In Fig. 3, we compare the numerically calculated radial mode profile (green) with the analytical solution (red). The analytical solution is given by (4). While the analytic oscillation (quasi) periodicity seems to agree reasonably well with the calculated one, the decay rates differ significantly. We attribute this difference to the fact that the profile (4) is
accurate only for small perturbations [19] while the index perturbations of the simulated structure are rather strong.

Figure 4 depicts the dependence of the resonance frequency (green) on the angular perturbation frequency. $\alpha_\theta$ and $\alpha_r$ are maintained fixed at 0 and 0 respectively. The x-axis indicates the number of holes in the first “necklace” (fig. 1c). While the resonance frequency is relatively insensitive to the angular perturbation frequency, the $Q$ of the resonator varies significantly when this frequency is changed. The $Q$ reaches a peak value of about $Q = 25,000$ around $l = 70$ and decreases significantly for both smaller and larger $l$. Two-dimensional simulations [19] showed that the $Q$ is expected to increase with $l$. We attribute this trend to the fact that smaller holes generate a more homogeneous angular perturbation which is closer to the ideal case of concentric rings. Therefore, we believe that the decrease in the $Q$ observed for $l > 70$, is a numerical artifact stemming from the limited resolution of the numerical scheme. The modal volumes of the structures with $l = 65$, 70 and 75 are respectively 3.8, 4.6 and 3.8 cubic wavelengths. It can therefore be seen that while the $Q$ is significantly affected by $l$, its impact on the modal volume is rather small.

As discussed in section II, the perturbation profile is determined by two parameters: $\alpha_\theta$, which determines the duty-cycle of the angular dependence of the perturbation and $\alpha_r$, which, roughly speaking, determines the duty cycle of the radial dependence of the perturbation. In particular, $\alpha_\theta$ and $\alpha_r$ represent generalized threshold levels that determine the transition from high-index to low-index. The values of $\alpha_r$ and $\alpha_\theta$ determine the size of the holes where the
larger $\alpha_0$ and $\alpha_r$, the smaller the holes. $\alpha_0$ and $\alpha_r$ affect the overall size of the holes which have opposite impact on the vertical and horizontal losses. Larger holes (smaller $\alpha_0$ and $\alpha_r$) reduce the in-plane radiation losses but also generate more Fourier components which are above the light-cone, and thus, increase the out-of-plane (vertical) scattering. Correspondingly, smaller holes (softer perturbation) reduce the vertical scattering but also the horizontal confinement resulting in larger in-plane losses for a fixed external radius of the reflector. Consequently, for a device with fixed external radius, there are optimal $\alpha_0$ and $\alpha_r$ for which the total $Q$ is maximal.

Figure 5(a) shows the dependence of the $Q$ and the resonance frequency on $\alpha_0$ while $\alpha_r$ is fixed at 0. A large $Q$ is found for $\alpha_0 = 0.1$. Figure 5(b) shows the dependence of the $Q$ and resonance frequency on $\alpha_r$ while $\alpha_0$ is fixed at 0. Unlike the angular perturbation, which is periodic in $2\pi/l$ (see Eq. (3)), the radial perturbation is not exactly periodic because it is determined by the oscillations of the appropriate Hankel function. Similar to $\alpha_0$, there is an optimal value for $\alpha_r$, in this case $\alpha_r$ is around 0, which is determined by the tradeoff between the horizontal and the vertical $Q$s. It should be emphasized that the optimal values for $\alpha_0$ and $\alpha_r$ stem from the fixed external radius of the Bragg reflector. Increasing the reflector radius would improve the horizontal $Q$ and would allow for larger $\alpha_0$ (softer perturbation).

Finally, we examine the impact of the effective index ($n_{\text{eff}}$) on the $Q$ and resonance frequency while fixing $l=65$, $\alpha_r=0$ and $\alpha_0=0.1$. $n_{\text{eff}}$ is a design parameter which stems from the reduction of the 3D problem to an equivalent 2D problem. To determine the holes position, the slab configuration is replaced by an equivalent 2-D structure with an effective index, $n_{\text{eff}}$, determined by the vertically guided mode of the slab. It is, therefore, important to verify the validity of this approximation by varying the value of $n_{\text{eff}}$ used in the design of the cavity. Figure 6 shows the impact of changing $n_{\text{eff}}$ in (3) on the $Q$ and resonance frequency. The maximal $Q$ is found for $n_{\text{eff}} = 2.86$, which is the effective index of the guided mode in the slab, thus indicating that the effective index approximation is valid and can be used for the design of such cavities.

4. Conclusion

We studied the impact of the various design parameters of circular PC cavities on their $Q$, modal volume and resonance frequency using 3D FDTD simulations. For a fixed size resonator, there is a clear tradeoff between the vertical and horizontal $Q$s manifested in optimal $\alpha_r$ and $\alpha_0$. We also found that increasing the angular (spatial) frequency of the perturbation generally increases the $Q$ up to a limit which, most probably, stems from
numerical errors generated by the limited resolution of the calculation scheme. We attribute this trend to the fact that higher perturbation frequencies generate smaller holes which reduces the local perturbation and the scattering losses, without affecting the radial coupling coefficient which confines the light in the central cavity. We also studied the influence of the effective index approximation used for the design procedure and found that the best $Q$ is attained when the actual slab effective is used for the design, thus validating the use of this approximation. Good agreement was found between the analytically and the numerically calculated radial field profile, even for relatively strong perturbation, indicating that the design and analysis method used here accurately describes the actual structure. The small number of design parameters and degrees of freedom (compared to PC defect cavities) allow for a thorough engineering of the cavity structure, yielding high $Q$s and small modal volumes.

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