High-Q cavity based on gradated one-dimensional photonic crystal*

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A high quality-factor (Q) cavity based on a one-dimensional (1D) photonic crystal with gradated elliptical holes was designed using FDTD simulation. Different gradient profiles of the mirror holes were found to correspond to different Q-values of the cavities. A simple strategy is proposed to construct high-Q cavities by using an S-shaped gradient profile for the elliptical holes' minor axes, such as a cosine function or Gaussian function. Using such a strategy, a Q value exceeding two million is obtained with only ten mirror holes in a cavity.

Keywords: photonic crystal, high-Q cavity, gradated cavities

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1. Introduction

High-Q cavities are important in opto-electronics because of their ability to enhance light-material interaction,[1–4] and to achieve nanobeam lasers[5–8] and nanobeam LEDs.[5] Nanocavities in two-dimensional (2D) photonic crystal (PhC) slabs can achieve both high quality factors (Q) and small modal volumes (V) approaching one cubic wavelength.[9,10] Noda *et al*. have experimentally demonstrated 2D PhC high-Q ($>$ 1 million) nanocavities with wide resonant wavelength ranges.[11] In order to reduce the footprint of the devices further, one-dimensional (1D) PhC cavities have recently emerged as a potential alternative to the slab-based 2D PhC[12,13] and cavities.[14] One-dimensional PhC cavities are not only high-Q candidates but also great platforms for integrated optics because they are optical waveguides themselves. Consequently, it is very useful to construct high-Q cavities based on 1D PhCs.

Many researchers have investigated this structure. Notomi *et al*. adapted the ideas of modified 2D PhC cavities into creating gradated 1D PhC cavities with ultrahigh Q (2.0×10^8) and wavelength-sized mode volume.[15] Zhang *et al.* demonstrated that 1D photonic crystal cavities supported both TE- and TM-polarized modes, each with a Q factor greater than one million and a mode volume on the order of a cubic wavelength.[16] Most of the research about 1D PhC cavities is based on silicon.[17–21] Meanwhile, other materials (such as silicon nitride, aluminum nitride and silicon dioxide) have also been investigated to form high-Q and low mode volume 1D PhC cavities.[22–24] Some high-Q cavities have been achieved in gradated 1D PhC waveguides by changing the distance between holes,[20] circular holes' radius,[25] and waveguide width.[5] These designs are compatible with normal optical waveguides. Harvard researchers proposed a theory that high-Q cavities could be achieved by creating cavity modes with a Gaussian-like attenuation profile.[14,26] In accord with this principle, we introduce a strategy to design such a cavity, which can greatly reduce the complexity of the design process. Following our designs, a 1D PhC cavity with a Q value exceeding two million and fewer than 10 period mirror holes can be achieved.

2. Design and simulation

2.1. Designing principles

The loss of 1D photonic crystal cavities ($1/Q_{\rm tot}$) has two main components, the radiation loss into free space ($1/Q_{\rm rad}$) and the coupling loss to the waveguide ($1/Q_{\rm wg}$). Their relationship is as follows:

$$\frac{1}{Q_{\rm tot}}=\frac{1}{Q_{\rm rad}}+\frac{1}{Q_{\rm wg}}. \tag{1}$$

Due to the band gap properties, $Q_{\rm wg}$ can be simply increased to almost infinity by arranging more periods in the 1D PhC structure. However, there is no deterministic method to increase $Q_{\rm rad}$ easily. Noda *et al.* investigated the Fourier transformation (FT) of the electric field inside the cavity, finding that large components inside the leaky region of the spatial FT spectra lead to large loss of radiation from the cavity.[9] Loncar *et al.* also found that $Q_{\rm rad}$ can be increased by minimizing the spatial Fourier harmonics of the cavity modes inside the light cone, which is achieved by creating a Gaussian-like attenuation profile.[26] These results indicate that soft confinement is the key to achieving a high-Q cavity. For 1D PhC cavities, gradated adjustment of the PhC holes is one of the most important methods to achieve soft confinement.

Our designs are basically gradated 1D PhC. We change the holes' shape from perfectly circular to elliptical. For the elliptical holes, the major axes are perpendicular to the waveg-

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uide and the minor axes are parallel to the waveguide. The minor axes decrease gradually when their positions approach the middle of the cavity (Fig. 1). This gradient profile can modulate the field distribution of the harmonic modes. There can be several gradient profiles, such as linear, cosine, and Gaussian.



Fig. 1. Structure of gradated 1D PhC cavity.

The period of the PhC is a and the width and thickness of the waveguide are $1.2a$ and $0.6a$, respectively. The indexes of the waveguide and background are 3.4 and 1.0, corresponding to silicon and air. All of the major axes of the elliptical holes' are $b = 0.36a$, and the minor axes of the two holes closest to the middle of the cavity are $0.5b$.

The linear gradient profile can be expressed as

$$R^i_{\text{minor}} = 0.5 + 0.5\frac{i}{N_x}. \tag{2}$$

The cosine profile is

$$R^i_{\text{minor}} = 0.75 - 0.25\cos\left(\frac{i}{N_x}\pi\right). \tag{3}$$

The Gaussian profile is

$$R^i_{\text{minor}} = 1.0 - 0.5\exp\left(-\frac{(i/N_x)^2}{2\sigma^2}\right), \tag{4}$$

where i indicates the i-th hole, progressing from the middle of the cavity to the feeding waveguide, R^i_{minor} is the i-th hole's minor axis, N_x is the total number of the holes in each side of the cavity, and σ indicates the shape of the Gaussian profile. The smaller the σ is, the sharper the profile is.

2.2. Simulation

The three-dimensional (3D) FDTD methods are used to simulate our designs. A free program Harminv developed by MIT is used to solve the high-Q cavity problem. A sum of finitely-many exponentially decayed sinusoids in a given bandwidth is used to fit the cavity modes' vibrations. This method is better suited to solving an ultrahigh-Q cavity than straightforwardly extracting fast-Fourier-transformation (FFT) peaks. In all of our calculations a normalized frequency unit of a/λ is used.

We calculated the cavity mode of the cosine profile with $N_x = 5$ using both the Harminv method and the transmission spectrum method in order to verify the agreement of the two methods. The reason for using the low Q cavity to do the verification is that the calculations for high-Q cavity transmission spectra are very time consuming. In Fig. 2, the upper colored graph shows the cavity mode field pattern with a frequency of 0.30198, while the lower line graph is the transmission spectrum of this cavity. The transmission at the cavity resonant frequency 0.30198 reaches 83.6%, higher than that of a 2D photonic crystal cavity. The obtained Q values are 6169 with the Harminv method and 6156 with the transmission spectrum method. Considering numerical errors of the calculations, which may cause fluctuation of the Q value, the results from two methods coincide well. In the following simulations, we use only the Harminv method to calculate the Q values of the cavities.

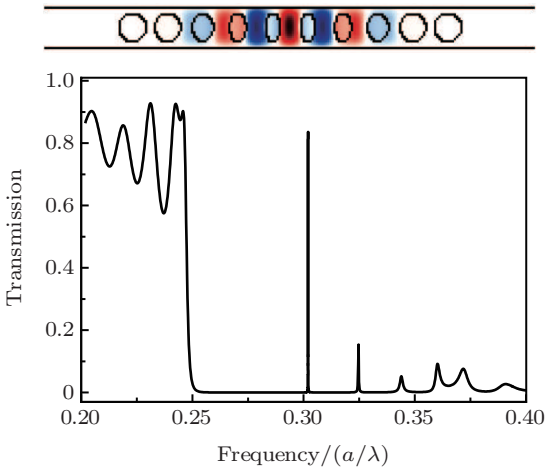


Fig. 2. (color online) Field pattern and transmission spectrum of cosine profile of $N_x = 5$.

As Figs. 3(a) and 3(c) show, for all of the gradient profiles, the cavity modes' frequencies decrease as the period number increases. The decrease of frequencies is due to the gradient profile of the minor axes. As the period number increases, minor axes of the holes near the center of the cavity become smaller. For example, in a linear gradient profile, the second hole's minor axis is 0.6, 0.55, and 0.525, when the period number is 5, 10, and 20, respectively. The shorter minor axes generate a bigger harmonic space in high-index material, which decreases the cavity-mode frequencies.

As the period number increases, the variations of the Q values are a bit complex. For a linear gradient profile, the logarithm of the Q value is directly proportional to the period number but the rate of increase is not large. For a cosine gradient profile, as the period number increases, the Q value first increases and it then decreases. The maximum Q value of 7.9×10^7 is obtained for 25 periods. For a Gaussian gradient profile, different σ structures make different profiles and Q value variation. The large σ profiles (e.g., $\sigma = N_x/0.5$) are similar to the linear profile, the middle σ profiles (e.g., $\sigma = N_x/2.0$) are similar to the cosine profile. The small σ profiles (e.g., $\sigma = N_x/3.0$) generate higher Q values for small period numbers, but as the period numbers increase, the Q values rise slowly. Gaussian profiles with σ being $N_x/3.0$, $N_x/2.5$, $N_x/2.0$, $N_x/1.5$ reach their highest Q values 9.0×10^7, 9.0×10^7, 8.5×10^7, and 7.4×10^7, for period numbers 35, 30, 25, 20, respectively (Fig. 3(d)). For a cosine profile, the cavity Q value can reach 2.4×10^6 with only 10 mirror holes, as Fig. 3(b) shows.

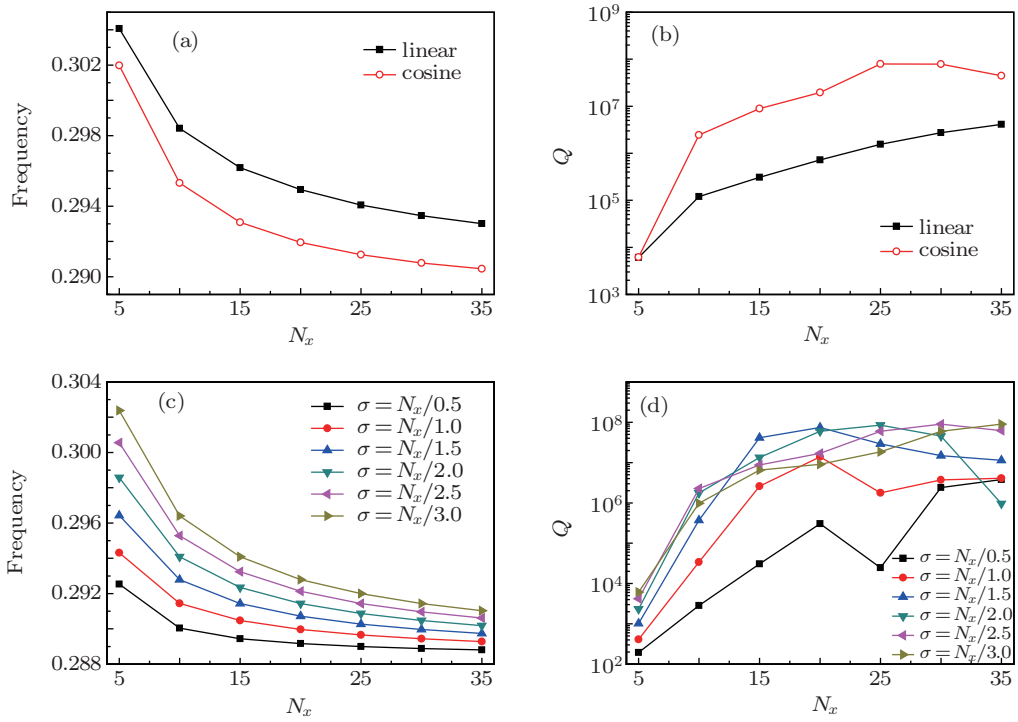


Fig. 3. (color online) Harmonic mode frequencies and Q values of cavities with different profiles. Linear profile and cosine profile (a) harmonic modes frequencies and (b) Q values. Gaussian profiles with different σ (c) harmonic modes' frequencies and (d) Q values.

A linear gradient profile can generate a higher Q mode than a traditional one-defect cavity. Cosine profiles and Gaussian profiles can even produce much higher Q values. The cosine profile is fixed, but for a Gaussian profile, different σ values introduce different gradation rates, which strongly affect the Q value. All of the profiles of the high-Q cavities have an S-shaped gradation rate of the minor axes; for example, the minor axes decrease from the middle cavity with a rate that is at first slow, then fast, and then slow, as Eqs. (3) and (4) describe.

3. Discussion

First, we analyze the modes in a linear gradient profile and cosine gradient profile of $N_x = 10$ to characterize a high-Q mode. There are many abrupt transitions in the mode field distributions along and inside the waveguide because of the index's sharp changes arising from the elliptical shape of the holes. So we use the mode field distributions along the side of the waveguide to analyze its Q value characteristics. A trigonometric function with Gaussian decayed amplitude $y = A\exp(-\xi x^2)\cos(2\pi x/T)$ is used to fit the simulation data. The mean square error and Q value of the cosine gradient profile are 0.056 and 2.4×10^6, while the mean square error and Q value of linear gradient profile are 0.080 and 1.2×10^5. The gradient profiles with lower mean square error of mode fields will correspond to higher Q values. From Fig. 4 we can see that the mode field distribution of a cosine gradient profile coincides better to the fitting function than that for a linear gradient profile. The suppressions of mode fields of a linear gradient profile are too large at the second side peak and too small at the third side peak. This indicates that the linear gradient profiles are not suitable enough to confine the mode softly. For the linear gradient profile, the minor axes vary linearly, while the cosine gradient profile has an S-shaped gradation rate.

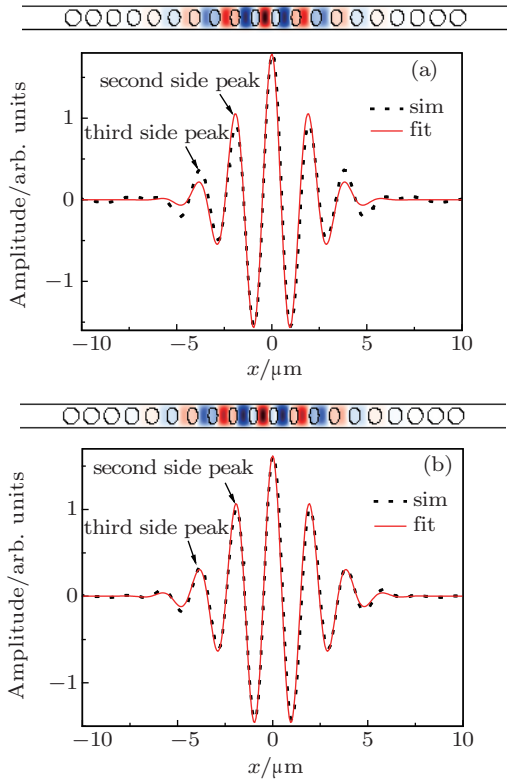


Fig. 4. (color online) Mode field distributions and fitting curves of (a) linear profile of $N_x = 10$, and (b) cosine profile of $N_x = 10$.

Two methods, which are the PhC band structure method and the index profile method, can be used to explain how the minor axes' gradient profiles affect the modes. The 1D PhC band structures change considerably as the holes' minor axes change. From Fig. 5 we can see that there are two main bands below the light line. Both bands drop with the shortening of the minor axes. For minor axes of $1.0b$ in Fig. 5(b), the higher and lower band edges are 0.381 and 0.265. For minor axes of $0.5b$ in Fig. 5(a), the higher and lower band edges are 0.288 and 0.244. The high bands go down more and the ranges of the band gaps shrink with the shortening of the minor axes. As the minor axes shorten, the effective index of the waveguide increases, which makes longer-wavelength modes available in the same period. From another point of view, because TE modes' energy is mainly kept in high index material rather than in the air, structures with shorter minor axes maintain more high-index material and confine more of the electric field inside.

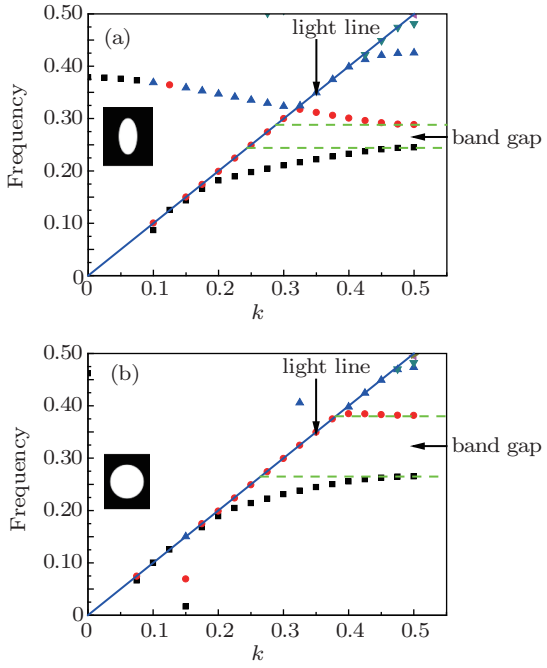


Fig. 5. (color online) Band structures with minor axis of (a) $0.5b$ and (b) $1.0b$.

The band structure changes also vary the reflection ratio. For the frequencies in the band gap, the reflection ratio of a certain 1D PhC structure has a positive correlation with the frequency's distance from the nearest band and the number of periods of the PhC. This means that for a given finite 1D PhC structure, the transmission is lower when the frequency is located inside the gap than when it is located near the band edge. Figure 6 shows the transmission of one-sided mirrors of different profiles. All of the transmission lines go down when the frequency is beyond the band edge. The cosine and linear profile mirrors' transmission lines are between the $0.5b$ and $1.0b$ situations. If a cavity mirror is designed with a linear or cosine gradient profile, then the reflection ratios also gradually change with the frequency position. This is the key point of soft confinement.[26]

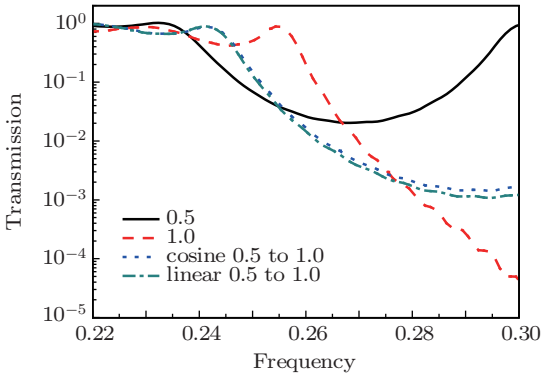


Fig. 6. (color online) One-sided mirror transmission of different profiles of $N_x = 5$. The values are the lengths of the minor axes of the holes.

The choice of $0.5b$ minor axes was mainly made because the harmonic mode ($f \approx 0.29$) is within the high band of PhC and near the band gap. As the mode field distributes along the waveguide, the minor axes become longer and the high band rises. Then, the mode frequency reaches the band gap and moves deeper into the band gap. The reflection ratio increases gradually along the waveguide. This is how the soft confinement and the high-Q cavity are made up. As Fig. 7 shows, with the same 10 side mirror periods, a linear profile in Fig. 7(a) confines light a little more strongly than a cosine profile in Fig. 7(b). The mode field distribution in the cosine profile can reach the sixth hole from the middle cavity, while that of linear profile can only reach the fifth hole. The confinements of the cosine profile are softer than those of the linear profile, and the Q value of the cosine profile is higher. But this is not the case that softer confinement is always better. The Gaussian profile with $\sigma = 0.5N_x$ in Fig. 7(c) has a larger mode field distribution area than that of the Gaussian profile with $\sigma = 3.0N_x$ in Fig. 7(d) because it has a slowly varying profile, so the reflection ratio also varies slowly along the waveguide. This means that the confinement in Fig. 7(c) is softer but its Q value is lower than that of Fig. 7(d). Because the confinement is too low, the light leaked to the feeding waveguide is not negligible.

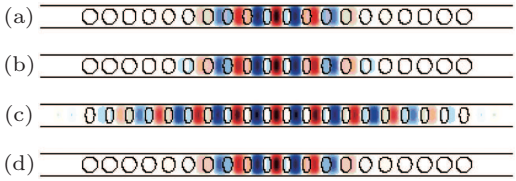


Fig. 7. (color online) Mode field distribution of (a) linear profile of $N_x = 10$, (b) cosine profile of $N_x = 10$, (c) Gaussian profile with $\sigma = N_x/0.5$ of $N_x = 10$, and (d) Gaussian profile with $\sigma = N_x/3.0$ of $N_x = 10$.

From another point of view, the index profile variation changes the harmonic space. From the cavity to the feeding

waveguide, the amount of mode energy distributed in the air varies and fields of different strengths are distributed in the holes' side walls. Whether for real devices or simulations, the side walls are primary locations of scattering loss. So the gradient index profile caused by the gradated shapes of the holes can gradually inhibit the cavity mode emission. A proper index profile can draw the mode profile toward the Gaussian-like attenuation profile, to achieve low radiation to the air and a high-Q cavity mode.

In this work, the designed 1D PhC cavity in normalized frequency can be applied in the optical communication region. For the center wavelength 1550 nm, the design in this work has a scale of $a = 470$ nm, $b = 0.36a = 170$ nm, and the elliptical holes' smallest curvature radius is 90 nm. These parameters are reachable with today's electron beam lithography.

4. Conclusion

In this work, a method of gradated elliptical holes is proposed to design a 1D PhC cavity. The structure is realized by changing the holes' shape from perfectly circular to elliptical in a no-defect holey waveguide, making the major axes perpendicular to the waveguide and gradually varying the minor axes, with an S-shaped profile such as a cosine function or Gaussian function. This 1D PhC cavity with an S-shaped Gaussian-like gradient index profile can achieve a high-Q cavity, and a short cavity (10 side mirror holes) with a relatively high Q value (more than two million). The simulations of photonic band-structure and the field distribution further verify the high-Q cavity. This design is compatible with normal optical waveguides that are suitable for future photonic integrated circuits.

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