Physical origin of the small modal volume of ultra-high-\(Q\) photonic double-heterostructure nanocavities

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Abstract. We have recently demonstrated the fabrication of ultra-high-\(Q\) photonic double-heterostructure nanocavities with \(Q\)-factors of almost 1 million and ultra-small modal volumes with dimensions of optical wavelengths. Here, we describe the physical origin of the small modal volume by analysing the (imaginary) dispersion relations of the mode-gap of photonic crystal (PC) waveguides, where the mode-gap effect is the fundamental principle by which photons are confined in the nanocavities. By expanding the real dispersion relations of the propagation modes of different PC waveguides into their complex form, we obtain the (imaginary) dispersion relations of the mode-gap. It is shown that the ultra-small modal volume originates from the unusual dispersion relation of the propagation mode of the PC waveguide and that it can be engineered by the geometric parameters of the waveguide. This is demonstrated experimentally by the fabrication of photon tunnelling structures and measurement of their transmission characteristics. These results reported here will be very useful for the realization of high-\(Q\) cavities with ultra-small modal volumes and their application to nanophotonics.

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1. Introduction

The strong confinement of photons in an ultra-small cavity with dimensions of the order of optical wavelengths [1, 2] is very important for the development of nanophotonic applications. For example, single-photon emitters [3] for quantum communication and computing, nanolasers [4], the stopping of light [5], atom trapping [6], ultra-small photonic filters [7], optical memories, bio- and chemical sensing can all be realized using nanocavities with high $Q$-factors. Although the potential of both Fabry–Perot [8] and whispering gallery [9] cavities for the above photonic applications has been studied, photonic crystal (PC) cavities are the most promising because of their extremely small modal volumes. Recently, an important design rule for the realization of high-$Q$ nanocavities in two-dimensional PC slabs has been proposed [1]: the electric field distribution of the cavity should have a Gaussian envelope function in order to minimize the out-of-slab leakage of photons.

Recently, the formation of a photonic double-heterostructure [2] (see figure 1(a)) has been shown to satisfy this design rule, and a $Q$-factor of 600 000 (see figure 1(b)) has been demonstrated experimentally [2]. We note that a $Q$-factor of almost 1 million has since been achieved using a photonic multi-step heterostructure [10]. The double-heterostructure consists of a PC core waveguide (PC$_2$ waveguide) placed between two PC cladding waveguides (PC$_1$ waveguides). Because the lattice constants of PC$_1$ and PC$_2$ differ ($a_1 < a_2$), photons with a specific energy can be confined within the core waveguide by the mode-gap effect of the cladding waveguides [11], and the electric field of photons confined within the PC$_2$ waveguide decays exponentially (evanescently) into the PC$_1$ waveguides. Even though the difference in lattice constants between the two waveguides is just 10 nm, the modal volume of the resulting cavity was found to be only $\sim 1.2(\lambda/n)^3$ [2] by three-dimensional finite difference time domain (3D FDTD) calculation, where $\lambda$ and $n$ are the wavelength of light in air and the refractive index of the slab, respectively.

In this paper, we describe the physical origin of this ultra-small cavity modal volume by analysing the mode-gap effect of PC waveguides. The dispersion relations of the two different types of waveguides described above are theoretically investigated. It is shown that the mode-gap effect (and thus the modal volume) can be engineered by selecting the geometric parameters of the waveguide. Furthermore, we investigate the mode-gap effects of the two waveguides experimentally.
Figure 1. (a) Schematic picture of a photonic double-heterostructure nanocavity constructed by connecting PC waveguides PC1 and PC2 with lattice constants $a_1$ and $a_2$, respectively. (b) Experimental results for a photonic double-heterostructure nanocavity, showing the resonant spectrum of the cavity over a wide range of wavelengths. The inset shows the near-field image observed using an infrared camera. Extremely narrow line-widths of 2.8 pm were obtained, corresponding to $Q$-factors of 600,000 (which is referred to [2]).

2. Theoretical results

2.1. Dispersion relations of PC waveguides (I)

Figure 2 shows the calculated electric field distribution in the photonic double-heterostructure nanocavity depicted in figure 1, where the lattice constants of PC1 and PC2 are $a_1 = 410$ nm and $a_2 = 420$ nm, respectively ($\Delta a = a_2 - a_1 = 10$ nm). As seen in the figure, the electric field is strongly localized within the PC2 waveguide (core region) and decreases exponentially, that is, evanescently, into the PC1 waveguide due to the mode-gap effect [11]. In order to understand how the electric field can be so tightly confined in the core waveguide when $\Delta a$ is only 10 nm, we need to investigate the characteristics of the evanescent wave.
The evanescent behaviour is determined by the imaginary part of the complex wavevector \( k \) of the PC\(_1\) waveguide mode. The complex wavevector can be derived from the dispersion relation of a propagation mode of the PC\(_1\) waveguide as follows. Figure 3(a) shows a schematic picture of a PC\(_1\) waveguide with lattice constant \( a_1 \). The radius of the air holes and the slab thickness are \( 0.29a_1 \) and \( 0.6a_1 \), respectively. The dielectric slab is assumed to be composed of silicon \((n = 3.4)\), which is transparent in the optical communication wavelength range of 1.3–1.6 \( \mu \)m. The width of the line-defect waveguide is \( W = \sqrt{3}a_1 \), which corresponds to one missing row of air holes in the \( \Gamma-J \) direction. Figure 3(b) shows the dispersion relation of a propagation mode of the PC\(_1\) waveguide calculated using the 3-DFDFTD method [12, 13]. The units of frequency \( f \) and wavevector \( k \) are \( c/a_1 \) and \( 2\pi/a_1 \), respectively, where \( c \) is the velocity of light in vacuum. A non-leaky propagating mode exists in the frequency range from 0.263 to 0.280 \( (c/a_1) \) [13], where the low and high frequency cutoffs are determined by the effects of the mode-gap and the light line, respectively [11, 14]. Because the dispersion relation of the propagation mode is purely real, the imaginary part of the wavevector is zero \((\text{Im}(k) = 0)\). On the other hand, the wavevector in the mode-gap region becomes complex because the electric field decreases evanescently. In order to derive the evanescent characteristics of the PC\(_1\) waveguide, we need to know the complex dispersion relation. The dispersion relations of various PC structures have been calculated by various methods [15, 16]. In this paper, we determine the complex dispersion relation of the PC waveguide using the analytic continuation method [17], that is, expansion of the real dispersion relation of the propagation mode into its complex form.

Before applying the analytic continuation method, the real dispersion function \( f(k) \) can be fitted using a Taylor’s series expansion of the term \((k - 0.5)\). Here, we consider only the even order terms since the dispersion relation is even at the Brillouin zone boundary \((k = 0.5)\). The fitted result is expressed as

\[
  f = 0.263 + 0.01 \times (k - 0.5)^2 + 2.5 \times (k - 0.5)^4 + 240 \times (k - 0.5)^6 
\]

and the fitted curve is shown by the red solid line in figure 3(b). As seen in equation (1), we have used not only the second order term \((k - 0.5)^2\) but also fourth and sixth order terms to fit the dispersion curve near the mode-edge frequency, \( f_0 = 0.263 \). This is because the slope of the
Figure 3. (a) Schematic picture of a PC$_1$ waveguide with lattice constant $a_1$ and width $W = \sqrt{3}a_1$. (b) The calculated dispersion relation of a propagation mode for panel (a). (c) The dispersion relation of the mode-gap obtained using the result of panel (b).

dispersion curve near the mode-edge is unusually small, which is attributed to the fact that the guiding mechanism of this waveguide is not due to refractive index guiding but to photonic band gap (PBG) guiding.

2.2. Dispersion relations of PC waveguides (II)

Next, the imaginary dispersion relation for the mode-gap region can be derived using the analytic continuation method by substituting the complex wavevector $k = 0.5 + iq$ into equation (1), where $q$ is the imaginary part of $k$ ($q = \text{Im}(k)$). The obtained dispersion curve in the mode-gap region is shown in figure 3(c) and is like a step function. Thus, even when the cavity frequency ($f_{\text{cavity}}$) is very close to the mode-edge frequency $f_0$, $q$ can have a relatively large value. For example, when the difference ($\Delta f$) between $f_{\text{cavity}}$ and $f_0$ is as small as $\Delta f = 0.0012c/a_1$ in the double-heterostructure cavity with $a_2 - a_1 = 10$ nm, $q$ is calculated to be $0.07(2\pi/a_1)$ and hence the penetration length ($1/2q$) is only $1.14a_1$. Such weak penetration into the PC$_1$ waveguide can quantitatively explain the small modal volume of the double-heterostructure cavity. We note that the exact value of the modal volume is obtained from the three-dimensional structure.

Next, we consider the dispersion relation of the PC waveguide shown in figure 4(a), which we refer to as the PC$_1'$ waveguide. The structure of this waveguide has the same geometric parameters as those of the PC$_1$ waveguide in figure 3(a) except for the width ($W' = 0.62 \times \sqrt{3}a_1$). The dispersion relation of a PC waveguide propagation mode is dependent on the width of the
The dispersion relation of the propagation mode of the PC waveguide was calculated using a similar procedure to that described above, and is shown in figure 4(b). It can be fitted as

\[ f = 0.2637 + 0.94 \times (k - 0.5)^2 \]  

(2)

Unlike in equation (1), the dispersion relation of this propagation mode can be fitted using only a second order term of \((k - 0.5)^2\). This is because the shape of the waveguide dispersion curve near the mode-edge at \(f_0 = 0.2637\) is simply parabolic, which is attributed to the fact that refractive index guiding is the relevant mechanism here, as in conventional dielectric waveguides.

Substituting \(k = 0.5 + iq\) into equation (2), we obtain the complex dispersion relation of the PC waveguide, which is plotted in figure 4(c). In this case, when \(\Delta f = f_0 - f_{\text{cavity}} = 0.0012c/a_1\), \(q\) has the much smaller value of 0.017\((2\pi/a_1)\). As a result, the penetration length of the mode propagating into the cladding waveguide with \(W = 0.62 \times \sqrt{3}a_1\) is 4.69\(a_1\), which is approximately four times longer than that for the waveguide with \(W = \sqrt{3}a_1\). This result indicates that the modal volume of the double-heterostructure nanocavity greatly increases when the waveguide mechanism changes from PBG guiding to refractive index guiding. Importantly, this qualitative relationship between the modal volume and the mode-gap characteristics of a PC waveguide indicates that it is possible to realize ultra-high-\(Q\) photonic nanocavities with smaller modal volumes.
Figure 5. (a) Schematic picture of a photon tunnelling structure fabricated for the experimental investigation of transmission characteristics due to the mode-gap effect of a PC1 waveguide. Here, the length $l$ of the PC1 waveguide is varied. (b) and (c) show SEM images of the fabricated photon tunnelling structures of a PC1 waveguide with width $W = \sqrt{3}a_1$ and a PC1′ waveguide with width $W' = 0.62 \times \sqrt{3}a_1$, respectively; the length of both waveguides is $l = 5a_1$.

3. Experimental results

3.1. Sample structure and fabrication

As discussed in the previous section, the evanescent characteristics of a PC waveguide due to the mode-gap effect are sensitive to the geometric parameters of the waveguide. The mode-gap effects obtained theoretically can be demonstrated experimentally by measuring the transmission characteristics of PC waveguides with different lengths, when these are comparable to the penetration lengths. Because it is somewhat difficult to measure the evanescent behaviour of PC waveguides directly, we fabricated heterostructures that enabled photon tunnelling, as illustrated in figure 5(a), and measured their transmission characteristics. The photon tunnelling structure consists of a PC1 waveguide sandwiched between two PC2 waveguides, where $a_1 < a_2$. The positions of PC1 and PC2 have been reversed compared to the photonic double-heterostructure in figure 1(a). Photons with a specific energy can tunnel through the PC1 waveguide due to evanescent coupling with the PC2 waveguide. The mode-gap effect of the PC1 waveguide can be estimated by measuring the transmission characteristics. The PC1 waveguides had lengths of a few $a_1$ lattice periods, whereas the two surrounding PC2 waveguides had lengths of several hundred $a_2$ periods, where $a_1$ and $a_2$ were set to 410 and 420 nm, respectively. In order to investigate the dependence of the mode-gap effect on the width of the waveguide, as discussed in subsections 2.1 and 2.2, PC1 and PC1′ waveguides with widths of $W = \sqrt{3}a_1$ and $W' = 0.62 \times \sqrt{3}a_1$ were fabricated. The width of the PC2(PC2′) waveguide was made proportional to that of the PC1(PC1′) waveguide, that is, either $\sqrt{3}a_2$ or $0.62 \times \sqrt{3}a_2$. The samples were fabricated on silicon-on-insulator (SOI) wafers, where silicon is transparent in the currently used optical communications wavelength range. The SOI wafer consisted of a 250 nm thick Si
Figure 6. Measured transmission spectra of photon tunnelling structures containing (a) PC1 waveguide with width $W = \sqrt{3}a_1$ and lengths $l = 10a_1$, $5a_1$ and $2a_1$, and (b) PC′1 waveguide with $W' = 0.62 \times \sqrt{3}a_1$ and lengths $l = 10a_1$, $5a_1$ and $2a_1$. The red and blue arrows indicate the mode-edge frequencies of the reference PC1 (PC′1) and PC2 (PC′2) waveguides, respectively, which were separately measured.
$W = \sqrt{3}a_1$, where the frequency $f$ is expressed in units of $c/a_1$, the unit frequency for PC$_1$, and the transmission intensity has been normalized by the maximum intensity in each individual transmission spectrum. The red and blue arrows represent the low frequency cutoff (mode-edge) of the PC$_1$ and PC$_2$ waveguides, respectively, which were measured using the reference samples.

The value of $0.264c/a_1$ for the PC$_1$ waveguide agrees well with the calculated cutoff frequency in figure 3(b). As seen in the transmission spectra of the PC$_1$ waveguide, the low frequency cutoff for the structure with $l = 10a_1$ almost coincides with that of the PC$_1$ waveguide reference sample with $l \sim 730a_1$. This indicates that even a PC waveguide with $l = 10a_1$ has a strong mode-gap (barrier) effect comparable to that of a PC$_1$ waveguide of semi-infinite length.

The spectra show that the low frequency cutoff decreases as the PC$_1$ waveguide becomes shorter, which can be interpreted as follows: when the length of the PC$_1$ waveguide approaches the penetration length of light propagating from the PC$_2$ waveguide into the PC$_1$ waveguide, the probability of photons tunnelling between the two PC$_2$ waveguides increases. We note that the transmission intensity decreases drastically near the low frequency cutoff, even for the PC$_1$ waveguide with the shortest length of $2a_1$. However, figure 6(b) shows that the transmission characteristics of samples with the narrower PC$_1'$ waveguide differ significantly. As typified by the result for $l = 10a_1$, the transmission decreases very smoothly near the low frequency cutoff (indicated by the red arrow), determined using the reference sample PC$_1'$ compared to that of the wider PC$_1$ waveguide. Even in the case of $l = 2a_1$, the mode-gap effect of the PC$_1'$ waveguide seems to disappear. In order to explain these experimental results, we have calculated the transmission spectra of the photon tunnelling structures. The transmittance ($T$) of a photon tunnelling structure is given by

$$T = e^{-2ql}$$

where we ignore the reflectance at the interfaces due to the mismatch between the modes of waveguides PC$_1$ (PC$_1'$) and PC$_2$ (PC$_2'$), $q$ is the imaginary part of the complex wavevectors obtained in figures 3(c) and 4(c), and $l$ is the length of the PC$_1$ or PC$_1'$ waveguide. The calculated transmittance spectra of the tunnelling structures with widths $W$ and $W'$ are shown in figures 7(a) and (b), respectively, for lengths $l = 2a_1$, $5a_1$, and $10a_1$. Here, the frequency has been obtained by substituting $q$ into the relevant equation (1) or (2). Comparing the spectra in the mode-gap region (low frequencies), it is observed that the transmission intensities of the structures containing the PC$_1$ waveguide are lower than those of the structures containing PC$_1'$ for the same values of length. This is because the value of $q$ for the PC$_1$ waveguide is larger than that of the PC$_1'$ waveguide. More importantly, the calculated transmittance of the structure containing the PC$_1$ waveguide drops steeply compared to that containing the PC$_1'$ waveguide—which agrees quantitatively with the experimental result of figure 6. This is because the imaginary dispersion relation of the mode-gap of the PC$_1$ waveguide is like a step function, as discussed in subsection 2.2.

We now discuss the experimental results of figures 6(a) and (b) in more detail, in particular the case of $l = 10a_1$ because the PC waveguides $l = 10a_1$ have enough mode-gap effect comparable to semi-infinite PC waveguides as explained above. The top of figure 8 shows the transmittance spectra of the tunnelling structures with $l = 10a_1$, where the transmittance is normalized by the transmission intensity at mode-edge frequency and the green dashed lines represent the noise level ($\sim 20$ dB) of our transmission measurement. A low transmission frequency range due to the mode-gap effect of the PC$_1$ (PC$_1'$) waveguide exists between the low frequency cutoffs of the reference PC$_1$ (PC$_1'$) and PC$_2$ (PC$_2'$) waveguides, while transmission intensity at frequencies lower than the cutoffs of the reference PC$_2$ (PC$_2'$) decreases by mode-gap.
effects of both PC\(_1\) (PC\(_1^\prime\)) and PC\(_2\) (PC\(_2^\prime\)). For simplicity, we consider the mode-gap effect of PC\(_1\) (PC\(_1^\prime\)) and investigate the frequency range between the cutoffs of the reference PC\(_1\) (PC\(_1^\prime\)) and PC\(_2\) (PC\(_2^\prime\)). Using equation (3), the value of \(q\) is expressed as

\[
q = \frac{-\ln T}{2(l/a_1)} \times \frac{1}{2\pi} 
\]  

where \(T\) is obtained from transmittance spectra of figure 8 and \(q\) is normalized by units of \(2\pi/a_1\). The results obtained from equation (4) are plotted at the bottom of figure 8. Although the values of \(q\) are limited to the noise level (∼20 dB) of the transmission measurement as shown by green dashed lines, it is seen that the value of \(q\) for the PC waveguide with width \(W = \sqrt{3}a_1\) increases drastically near cutoffs of PC\(_1\) compared to that for the PC\(_1^\prime\) waveguide with width \(W' = 0.62 \times \sqrt{3}a_1\). This result shows clearly the difference between the mode-gap effects of the PC\(_1\) and PC\(_1^\prime\) waveguides. Figure 9 shows the comparison of the experimental (red solid lines) and theoretical results (black dashed lines) (here, the experimental result of \(W' = 0.62 \times \sqrt{3}a_1\) is shifted toward a lower frequency by approximately 3% with respect to the theoretical curve of figure 4). As seen in the figure, the experimental results are in good agreement with the theoretical results, in particular the result of \(W' = 0.62 \times \sqrt{3}a_1\). If the noise level of the transmission measurement is reduced to approximately 50 dB, it is expected to obtain the values of \(q\) over a wider frequency range. Nevertheless, the transmission characteristics and \(q\) values shown
Figure 8. (a) and (b) Transmittance (top) and the estimated $q$ (bottom) of the PC$_1$ waveguide with width $W$ and a PC$'$$_1$ waveguide with width $W'$, respectively. Here, green dashed lines represent the noise level of our transmission measurement.

Figure 9. Comparison of experimental (red solid lines) and theoretical (black dashed lines) of (a) PC$_1$ waveguide with width $W$ and (b) PC$'$$_1$ waveguide with width $W'$. Here, the green dashed lines represent the noise level of our transmission measurement.

in figures 6–9 demonstrate clearly that mode-gap effects can be engineered by the geometry of a PC waveguide. These experimental results give important guidelines for optimizing the design of high-$Q$ nanocavities with small volumes, and thus enhancing the efficiency of photon manipulation [19].
4. Conclusions

In summary, we have investigated the physical origin of the small modal volumes of photonic double-heterostructure nanocavities where photons are confined by the mode-gap effect of a PC waveguide. By expanding the real dispersion relation of the propagating mode of the waveguide, we have theoretically obtained the imaginary dispersion relation of the mode-gap. By comparing the mode-gap effects of different PC waveguide structures, it has been shown that the small modal volume of the cavity originates from the unusual dispersion relation of the PC waveguides near the mode-edge, and the modal volume can be engineered by the geometric parameters of the PC waveguides. Furthermore, the mode-gap effects of two different PC waveguides have been investigated experimentally by fabricating photon tunnelling structures and measuring their transmission. The experimental results demonstrate clearly the engineered mode-gap effect of a PC waveguide. We believe that the results reported here will be very useful for the realization of more sophisticated nanocavities and components for nanophotonics.

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