Calculation of propagation loss in photonic crystal waveguides by FDTD technique and Padé approximation

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Abstract

The propagation losses in single-line defect waveguides in a two-dimensional (2D) square-lattice photonic crystal (PC) consisted of infinite dielectric rods and a triangular-lattice photonic crystal slab with air holes are studied by finite-difference time-domain (FDTD) technique and a Padé approximation. The decaying constant $\beta$ of the fundamental guided mode is calculated from the mode frequency, the quality factor ($Q$-factor) and the group velocity $v_g$ as $\beta = \omega(2Qv_g)$. In the 2D square-lattice photonic crystal waveguide (PCW), the decaying rate ranged from $10^3$ to $10^7$ cm$^{-1}$ can be reliably obtained from $8 \times 10^3$-item FDTD output with the FDTD computing time of 0.386 ps. And at most 1 ps is required for the mode with the $Q$-factor of $4 \times 10^{11}$ and the decaying rate of $10^{-7}$ cm$^{-1}$. In the triangular-lattice photonic crystal slab, a $10^5$-item FDTD output is required to obtain a reliable spectrum with the $Q$-factor of $2.5 \times 10^8$ and the decaying rate of 0.05 cm$^{-1}$.

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Recently, the photonic crystal waveguides (PCWs) become very attractive in integrated optics because of advantages in confinement of electromagnetic wave by the photonic band gap (PBG) effect, which may result in very low propagation loss in not only straight waveguides but also sharp bends [1–6]. The PCW coupling to photonic crystal (PC) microcavity also attracts great interest for fabricating ultrasmall channel add-drop functional devices [7–9]. Propagation loss is a key factor in designing a PCW and it is related to the confinement of guided modes in the PCW. Many methods have been proposed to analyse the propagation loss in both 2D and 3D PCWs. Morand et al. [10] applied transmission line matrix to investigate the loss of guided mode in PC slab.

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Andreani and Agio [11] used the guided-mode expansion to quantify the level of intrinsic losses and analysed their dependence on the structure parameters. More recently, Li and Ho [12] analysed the loss of the PCW in 2D PC with a finite wall thickness by a transfer-matrix method. In the calculation, the decaying rate was usually obtained by evaluating the temporal decay of a single eigenmode in the PCW [11,12].

2D-FDTD with effective index method and the full 3D-FDTD were also applied to analyse the loss of PCW [5,13–15]. The FDTD technique [16] is an accurate and powerful numerical simulation tool, and it can easily deal with complicated structures. All solutions in an interesting frequency range can be obtained in a single FDTD simulation, and the decaying constant \( \beta \) of guided modes can be calculated from the mode frequency, the \( Q \)-factor and the group velocity \( v_g \) as

\[
\beta = \frac{\omega}{2Qv_g}.
\]

In order to obtain mode frequencies and \( Q \)-factor, the FDTD output in time-domain must be transformed into frequency-domain. The natural selection is the fast Fourier transform (FFT), however, the resolution of the FFT scheme is inversely proportional to the total persistence time of the FDTD iteration, i.e., the product of the iteration number and the time step. The time step of the FDTD technique is limited by the Courant limit, so the FDTD iteration number is required very high. If the propagation loss is very weak (i.e., high \( Q \)-factor for the guided modes), a very long time simulation is necessary for FFT to obtain accurate mode \( Q \)-factors and frequencies, which is a heavy burden on computer power and memory, especially in 3D simulation.

Recently, we applied a Padé approximation with Baker’s algorithm for calculating the mode frequencies and \( Q \)-factors [17,18] from the FDTD output, and found that the method is easy to manipulate and can save more computation time than the FFT/Padé approximation, especially for the cavity with nearly degenerate modes. In this article, we use FDTD technique combined with the Padé approximation to analyse the propagation loss in the PCW. Two-dimensional PC consists of infinite dielectric rods arrayed in a square lattice and 2D PC slab waveguides with air holes arrayed in a triangular lattice are numerically simulated to investigate the waveguide loss. The Padé approximation with Baker’s algorithm [17] are used to obtain the field spectrum from the FDTD time series output, and then the propagation losses are calculated from the \( Q \)-factor and the group velocity of the guided mode. For the 2D square-lattice PCW, the FDTD computing time is about 0.386 ps at the decaying rate of \( 10^3 \cdot 10^{-4} \) cm\(^{-1}\), which is corresponding to \( 8 \times 10^3 \)-item FDTD output. And the required FDTD computing time reaches 1 ps for the mode with \( Q \)-factor of \( 4 \times 10^{11} \) and the decaying rate of \( 10^{-7} \) cm\(^{-1}\). In the triangular-lattice photonic crystal slab waveguide, a \( 10^4 \)-item FDTD output is required to obtain reliable spectrum with the \( Q \)-factor of \( 2.5 \times 10^9 \) and the decay rate of 0.05 cm\(^{-1}\).

The 2D PC with dielectric cylinders in air arrayed in a square lattice [12] are considered with refraction index \( n = 3.4 \) and radius \( r = 0.18a \), where \( a \) is the lattice constant. By removing a row of dielectric cylinders along the \( \Gamma-X \) direction, we can create a PCW with the sketch map shown in the inset of Fig. 1, where the PC structure at either side of the waveguide has finite periods. Only band gaps for \( E \) polarization (electric fields lie along the cylinders) exist in this structure. So we only consider the propagation of electromagnetic wave with \( E \) polarization. The region between the two black lines in the insert of Fig. 1 is

![Fig. 1. Dispersion relations of \( E \) polarization for the square lattice PCW in \( \Gamma-X \) direction are plotted as the filled circles. The geometry of the waveguide is shown in the inset. The gray areas are the projected band structure of the perfect square PC.](image-url)
a supercell chosen in the FDTD simulation. Because of the translational symmetry of the waveguides, the periodic boundary conditions satisfying the Bloch theorem is used at the boundary perpendicular to the direction of the waveguide. The corresponding period term is $\exp(ika)$, where $k$ is wave vector and $a$ is the period in the direction of propagation. At the boundary parallel to the direction of waveguide, perfectly matched layer (PML) absorbing boundary conditions [19] are applied to terminate the computation window. Because the whole structure has mirror symmetry with respect to the waveguide axis, we can add even or odd symmetry conditions to the electric field components at the waveguide axis to excite the even and odd modes, respectively. At the same time, the symmetry conditions reduce the calculation domain to a half. The Gaussian function modulated cosine impulse is added to the field at a point inside the waveguide as an exciting pulse, which covers the interesting frequency range. The time variations of field component in some selected points inside the computation window are recorded as the FDTD output. Then we calculate the field spectrum from the FDTD output by the Pade approximant and get the mode frequency $\omega$ and $Q$-factor from the field spectrum. In the calculation of spectrum, any component of electric field or magnetic field can be used and the same results can be obtained.

The dispersion relation of the 2D PCW is shown in Fig. 1 with the filled circles corresponding to calculated guided mode. The horizontal axis is the wave vector in $TX$ direction in the reduced Brillouin zone, and the grey areas are the projected bands. The guided modes are localized in the waveguide due to the PBG effect. The gap centres at frequency $\omega = 0.37 \times 2\pi ca$, which corresponds to the free-space wavelength of 1.55 $\mu$m at $a = 0.57 \mu$m. The decaying rate $\beta = \omega d(2Qv_g)$ is plotted in Fig. 2 versus the mode frequency $\omega$, where the group velocity $v_g$ is calculated from dispersion curve in Fig. 1. The losses decrease with the increase of the mode frequencies and suddenly increase at the frequency of $0.45 \times 2\pi ca$, which approaches the region of the PC states, and the obtained decaying rates agree very well with [10]. An 8000-item FDTD output is requested to obtain a stable field spectrum for $Q$-factor ranging from 100 to $1 \times 10^7$. The corresponding FDTD computing time is 0.386 ps, and the lowest decay rate is $10^{-4}$ $\text{cm}^{-1}$. In contrast, we can only get field spectrum with the resolution of $2.4 \times 10^{11}$ Hz from the above FDTD output by FFT, and obtain the reliable value of $Q \sim 10^3$ at the wavelength of 1550 nm. Guided modes with much larger $Q$-factor need longer FDTD output series. When the $Q$-factor reaches $4 \times 10^{11}$ at $k = 0.7 \times \pi / a$ and $\omega = 0.429 \times 2\pi ca$ as $N = 7$ ($N$ is the layer number of the dielectric cylinders aside the waveguide), the corresponding decaying rate is $10^{-7}$ $\text{cm}^{-1}$, which requires a 20,000-item FDTD output for obtaining a stable field spectrum. In Fig. 3, we show the spectra intensity of guided mode at $k = 0.7 \times \pi / a$ and $\omega = 0.429 \times 2\pi ca$ with $Q$-factor $4.5 \times 10^8$ at $n = 5$. The spectra obtained by the Padé approximation from the 8000, 9000, 10,000, 11,000 and 12,000-item FDTD outputs are shown in Fig. 3(a)–(e), respectively. And the spectrum obtained by the FFT method from the 214-item FDTD output is shown in Fig. 3(f). The results show that 12,000-item FDTD output is required for obtaining smooth field spectrum by Padé approximation. The field spectrum obtained from FDTD output longer than 12,000-item is stable and can fit to the Lorentzian pattern very well. The wide spectrum centred at $\omega = 0.37 \times 2\pi ca$ in Fig. 3(f) is the spectrum of the exciting pulse. To obtain the...
Q-factors from the spectrum calculated by the FFT method is almost impossible because it requires a very long FDTD output series. In our calculation, the length of FDTD output needed to obtain smooth and steady spectrum is related to the mode Q-factor and interval between the modes. The longer output is needed for a very large Q-factor and narrow mode interval.

The more practical PCW structures are the PC slab waveguides, which have 2D periodic dielectric structures of finite height and strong index confinement in the third dimension. A PC slab with refractive index \( n = 3.4 \) and drilled air holes with radius of \( r = 0.3a \) in a triangular lattice pattern are considered, where \( a \) is the lattice constant. Above and below the slab are air claddings for strong confinement of light in the slab. The thickness of the slab is chosen to be \( D = 0.6a \). The PCW is introduced by filling a row of air hole along the nearest neighbor in the \( \Gamma-K \) direction. The structure of PC slab and the first Brillouin zone are shown in Fig. 4(a) and (b). The photonic band structure of complete PC slab is calculated by 3D-FDTD method. Only the TE-like mode is considered in this paper, whose electric field is symmetric about the \( x-y \) plane. So a symmetric boundary condition is set at \( z = 0 \) plane, only the upper half \((z \geq 0)\) of a unit cell is used in numerical calculation. In order to deal with the infinite extend of the air claddings, we imposed PML absorbing boundary condition [19] at \( z = 3.3a \). When we deal with the \( \Sigma \) and \( T \) points, we impose additional boundary conditions as [20]. In the calculation, symmetric and antisymmetric boundary conditions are imposed to electric field at \( y = 0 \) for points like (along \( M-K \) direction), respectively, because the mirror symmetry about \( y = 0 \) only changes the wave vectors along \( M-K \) by integral multiple of reciprocal lattice vector. So a quarter of unit cell is enough for the FDTD calculation. These considerations not only reduce the numerical task but also classify the guided mode by the

Fig. 3. Intensity spectra obtained by the Padé approximation from 8000, 9000, 10,000, 11,000 and 12,000-item FDTD outputs at \( n = 5 \) are shown in (a)–(e), respectively. The spectrum obtained by the FFT method from the \( 2^{14} \)-item FDTD output is shown in (f), where the main peak is the field spectrum of the exciting source. The range of frequency shown in (a)–(d) is \((0.428789104-0.428789110) \times 2\pi\).
spatial symmetry. In the numerical simulation, the spatial step is set to be $0.04a$ and $a = 0.5 \, \mu\text{m}$. For the sake of Padé approximation, only a 2000-item FDTD output is required to obtain a reliable spectrum for the perfect 2D PC slab. The photonic band structures are shown in Fig. 5, with the even (open circles) and odd (solid circles) modes for wave vectors along $\Gamma$–$K$, $\Gamma$–$M$ and $M$–$K$ classified by symmetry properties of electric field about $x = 0$, $y = 0$ and $x = 0$, respectively. The thick solid line is the light line, above which PC states may be diffracted to the radiation field in free space. We can see a gap exists from frequency $0.256c/a$ to $0.336c/a$. When a line defect waveguide is introduced, guided modes may appear in this gap.

Filling a row of air hole along the nearest-neighbor $\Gamma$–$K$ direction for the above PC slab, we can have a PC slab waveguide. We consider the propagation loss for the PC slab waveguide with five rows of holes in each side as shown in the inset of Fig. 6. Because the structure is symmetric to the axis of PCW along $x$-axis and wave vector along $\Gamma$–$K$ is hold by the mirror reflection operation about $x$-axis, we can impose symmetric and antisymmetric boundary condition to electric field at $x$-axis. The odd mode whose electric field is antisymmetric to $x$-axis is just the fundamental TE-like mode of the PCW. Due to the translational symmetry of the PCW, we choose a supercell marked by the broken lines in the inset of Fig. 4.

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Fig. 6 in the calculation. The Bloch boundary condition is imposed at two sides parallel to \(y\)-axis. PML boundary conditions are imposed at sides parallel to \(x\) and \(z\)-axis. The distance between the slab waveguide and PML boundary perpendicular to the \(z\)-axis is chosen to be 3\(a\) to ensure the accuracy of \(Q\)-factors. The dispersion relation of fundamental mode and the decay constant \(\beta\) is shown in Fig. 6. We can see that the frequency of the fundamental guided mode decreases with the increasing wave vector \(k\) and have very low group velocity at the edge of first Brillouin zone of PCW. The lowest normalized guided mode frequency is about 0.282 at wave vector \(k = 1.0\), which is a little different from the result in [15] (in [15], \(f_{\text{min}} = 0.265\)). Because the limit of speed and memory of our Dell workstation, the spatial step is set to be 0.04\(a\) in our calculation. When the spatial step is set to be 0.02\(a\), the normalized mode frequency obtained is 0.271, but the calculation time is very long. From the dispersion relation in Fig. 6, we can see that the guided mode with \(k < 0.6\pi/a\) is in the light cone and the diffraction to the radiation field in free space causes the out-of-plane loss. The guided mode with \(k > 0.6\pi/a\) is below the light line and in the photonic band gap. The corresponding guided mode is confined in the waveguide in the slab plane by PBG effect and in \(z\)-direction by the strong index confinement, so the propagation loss is very low in this range. As shown in Fig. 6, the decaying constants above the light line are 100–2000 times larger than those below. And the decaying constants are around 1 cm\(^{-1}\) when \(k = (0.65–0.8)\pi/a\), which do not decrease with the increasing wave vector as in Fig. 2. As \(k = (0.65–0.8)\pi/a\), the \(Q\)-factors of guided modes are almost 100 times lower than that at \(k = 0.9\pi/a\), and group velocities are about 10 times larger. The largest \(Q\)-factor reaches \(2.5 \times 10^8\) and \(\beta = 0.05\) cm\(^{-1}\) at \(k = 0.9\pi/a\). The loss of the guided modes below the light line with \(k\) around 0.9\(\pi/a\) is sub-0.1 cm\(^{-1}\), which is limited by finite PC walls, even the vertical scattering loss may be zero. This can also be seen in Fig. 2, where the decay constant \(\beta\) of guided mode (\(f = 0.35 \times c/a\), \(n = 5\) and \(a = 0.5\) \(\mu\)m) is about 0.1 cm\(^{-1}\). A 10,000-item FDTD output is required to obtain a reliable spectrum by the Padé approximation for the PC slab waveguide. And the propagation losses of multiple modes can be obtained from a single FDTD simulation. However, in Kuang’s [15] calculation of the vertical radiation loss, at least 30,000 time steps

![Fig. 7. Refractive index distribution of PCW in \(z = 0\) plane (a), where white region is air hole. Field distribution of \(H_y\) in \(z = 0\) plane for (b) antisymmetric TE-like mode at \(f = 0.282\) and (c) symmetric TE-like mode at \(f = 0.310\). Field distribution of \(H_z\) in \(x = 0\) plane for (d) antisymmetric TE-like mode at \(f = 0.282\) and (e) symmetric TE-like mode at \(f = 0.310\). The black solid lines in these figures indict the symmetric plane. The corresponding wave vector is \(k = \pi/a\) in (b)–(e).](image-url)
are needed to obtain a side-mode suppression ratio larger than 57 dB and a bandwidth of less than 0.005 in normalized frequency.

Finally, we excite a single guided mode at \( k = \pi/a \) with corresponding symmetry boundary condition by a narrow Gaussian pulse and show the field distribution in Fig. 7. Fig. 7(a) is the refractive index distribution of PCW in \( z = 0 \) plane, where white region is air hole. The field distributions of \( H_z \) in \( z = 0 \) plane for antisymmetric mode at normalized frequency \( f = 0.282 \) and symmetric one at \( f = 0.310 \) are shown in Fig. 7(b) and (c), respectively. For the antisymmetric and symmetric TE-like mode, the electric field is antisymmetric and symmetric to \( y = 0 \) plane, respectively, and is symmetric to \( z = 0 \) plane. And the symmetric behavior of magnetic field is contrary to the electric field. In Fig. 7(d) and (e), we plot the field distribution of \( H_z \) in \( x = 0 \) plane for the antisymmetric mode at \( f = 0.282 \) and symmetric mode at \( f = 0.310 \), respectively.

In conclusion, we have investigated the propagation loss in single-line defect waveguides in 2D square-lattice photonic crystal consisted of infinite dielectric rods and in triangular-lattice photonic crystal slab with air holes by FDTD technique and a Padé approximation. The symmetry boundary conditions are used in the simulation, which save the numerical task and classify the guided mode by the spatial symmetry. In both cases, the decaying rate of guided modes with \( Q \)-factors over \( 10^8 \) can be reliably obtained from very short FDTD output. And the requested length of FDTD output is almost independent on the \( Q \)-factor as \( Q \)-factor ranged from 100 to \( 1 \times 10^7 \). The results show that the numerical simulation by FDTD technique and Padé approximation is accurate and can greatly release the burden on computer power and memory.

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