Resonant modes of two-dimensional photonic bandgap cavities determined by the finite-element method and by use of the anisotropic perfectly matched layer boundary condition

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The finite-element approach to the eigenmode analysis of a photonic bandgap cavity by use of an anisotropic perfectly matched layer absorbing boundary is presented. This method rigorously calculates the resonant frequency, the field pattern, and the quality factor of the resonant mode of a finite-sized cavity in free space. The validity of the approach is examined through its application to two-dimensional photonic bandgap cavities. Analyses of numerical error for the resonant frequencies and the quality factor of the cavities demonstrate the accuracy and reliability of our approach, which used nonuniform grids, higher-order elements, and the perfectly matched layer. Far-field patterns of the resonant modes were obtained by simple transformation. Because the perfectly matched layer can represent the real boundary condition well, cavities of any size and shape can be analyzed with the desired accuracy. © 1998 Optical Society of America [S0740-3224(98)00908-4]

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1. INTRODUCTION

In recent years, photonic bandgap materials have attracted attention because they can control spontaneous emission and because of their applications to zero-threshold lasers, efficient light-emitting diodes, and wavelength-scale light-bending waveguides.1–3 Following the initial searches for dielectric structures with photonic bandgaps,4–6 interest has been focused on structures that are manufacturable in the optical region of the spectrum, on metal structures for applications in the microwave region, and on new cavity structures7–12 and atom–cavity interactions based on photonic bandgap cavities. Theoretically, the plane-wave expansion method is used as a standard tool for bandgap diagrams of photonic crystals.4–6 For resonant frequencies and field patterns of defect modes, the supercell method is mostly used.8,11–13 The real-space Green’s function method has also been used to find resonant frequencies of defect states.14,15 The oscillating dipole method was employed by other researchers to obtain resonant frequencies and field patterns.16,17 The quality factor, the coupling efficiency, and the transmittance were calculated by the finite-difference time-domain (FDTD) method.10–12,18

For finite-thickness layers, the transfer matrix method is frequently used for transmittance calculation.19 For a study of localiton, a multiple-scattering method employing the boundary integral was used.20,21 Experiments have been performed mainly in the microwave region. Recently, successful fabrications in the optical wavelength scale were also reported.22,23

For photonic bandgap cavities, the supercell method and the FDTD method are used mainly to investigate the properties of defect states in the frequency and time domains, respectively.5–13 Resonant frequencies and field patterns of the modes are usually calculated by the supercell method, which reveals polarization characteristics and symmetry properties of the modes.11 However, the Q factors of the cavity are calculated by the FDTD method, which determines the temporal behavior of the modes. This approach has been used to study the properties of strongly localized defect states or cavities. However, an impurity band, which is an artifact that is due to the interaction between defects in the adjacent supercells, appears when this method is used.9 This impurity band becomes nontrivial for small cavities. Moreover, the field, especially around the edge of the cavity, can be quite different from that of the real finite-sized cavity in the periodic boundary condition. Therefore the corresponding far field cannot be determined reliably. In fact, if one wishes to obtain the far-field pattern by the FDTD method, the scattering field pattern is needed. However, it is generally more difficult to obtain the far-field pattern by this FDTD method than by direct transformation of the field pattern.11,18,24 In addition, the difference relations in the FDTD method generate errors that are due to numerical dispersion, which limits the overall size of the structure.18,24 When the shape of the grid does not conform to the shape of a real material such as a circular rod, additional errors can be produced.24 As experimental techniques to fabricate small cavities are improved, a more rigorous method, which is free from these drawbacks, will be required.
In this paper we present a more accurate method based on the finite-element method (FEM) with the perfectly matched layer (PML) numerical absorbing boundary condition.\textsuperscript{25,26} Although the FEM is widely used for eigenmode analyses of electromagnetic waveguides and resonators with metal enclosures,\textsuperscript{27} the rigorous treatment of unbounded cavity structures draws attention again following the recent introduction by Berenger of the PML concept in the FDTD method.\textsuperscript{25} The PML is a nonphysical material that does not reflect the incident propagating wave independent of incident angle, frequency, and polarization. The propagating wave decays exponentially inside the PML. Sacks et al.\textsuperscript{28} developed an anisotropic PML that is easy to implement in the FEM and applied it to the computation of far-field radiation patterns of a dipole antenna. In our previous study we used the anisotropic PML concept to formulate the finite-element eigenvalue problem for open resonators, and its validity was examined by its application to one-dimensional resonators.\textsuperscript{28}

This method has several advantages. First, it deals with actual finite-sized cavities embedded in free space, in contrast to the infinitely periodic cavities assumed in the supercell method. Thus a more accurate field pattern along the boundary of the cavity as well as the field near the defect can be obtained by use of this method. The various cavity structures can be analyzed not only for the strongly localized state but also for the defect state near the boundary. Second, resonance properties including resonant frequencies, \( Q \) factors, and field distributions can be obtained simultaneously by simply solving the eigenmatrix equations applying the common boundary conditions only once, whereas other methods cannot generate these properties all at once. For example, the resonant frequency with the field pattern of the mode is calculated with the supercell method, assuming a periodic structure, whereas the \( Q \) factor is obtained independently by the FDTD method dealing with a nonperiodic finite-sized cavity. Finally, our approach, which uses higher-order elements and an appropriate mesh that conforms to the shape of the boundary, can greatly reduce the numerical errors that are due to numerical dispersion and the staircase approximation.\textsuperscript{24} The PML also provides a systematic way to reduce numerical errors that originate from the reflected waves at the boundaries. In addition, our method can treat boundary surfaces of various materials properly and effectively. For example, this method is expected to be powerful for analyses of metallic structures for which artificial surface states become troublesome.\textsuperscript{29} It is also advantageous that one can handle complicated structures with a relatively small number of divisions or elements by following the adaptive mesh-generation scheme.\textsuperscript{30} Furthermore, one can study lasing characteristics just by assigning a complex refractive index to the structure in this formulation.

We analyzed a two-dimensional (2-D) photonic bandgap cavity based on a square lattice\textsuperscript{11} to obtain various cavity parameters. We present the numerical errors associated with finite-element discretization and the reflection from the PML as a guide in selecting appropriate parameters to achieve the desired accuracy. We calculated the far-field pattern of the resonant mode of the cavity by transforming the field around cavity boundaries. Inasmuch as the PML faithfully represents the free space surrounding the cavity, we argue that the far-field pattern, which is an important observable parameter in laser experiments, can be obtained with accuracy by our method. Our results are compared with those from the supercell method and the FDTD method when necessary.

2. THEORY

A. Finite-Element Method with Anisotropic Perfectly Matched Layer

A 2-D photonic bandgap cavity with infinitely long rods is considered as a 2-D dielectric system, as shown in Fig. 1, and it is governed by the source-free Maxwell equations,

\[
\nabla \times \mathbf{E} + j \omega \mu_{r} \mathbf{H} = 0, \\
\nabla \times \mathbf{H} - j \omega \varepsilon_{r} \mathbf{E} = 0, 
\]

where \([\varepsilon_{r}]\) and \([\mu_{r}]\) are the relative permittivity and permeability of the medium, respectively, and \(\exp(j \omega t)\) is assumed for time dependence. \(\varepsilon_{0}\) and \(\mu_{0}\) are set to 1. The constants \([\varepsilon_{r}]\) and \([\mu_{r}]\) are assumed to be complex diagonal tensors of the form

\[
\begin{bmatrix}
\varepsilon_{xx} & 0 & 0 \\
0 & \varepsilon_{yy} & 0 \\
0 & 0 & \varepsilon_{zz}
\end{bmatrix},
\begin{bmatrix}
\mu_{xx} & 0 & 0 \\
0 & \mu_{yy} & 0 \\
0 & 0 & \mu_{zz}
\end{bmatrix}.
\]

We derive the formulation that permits diagonally anisotropic permeabilities to deal with unbounded field problems by the PML method, which we explain below. We complete the formulation of the field problems by specifying boundary conditions. An absorbing boundary condition (ABC) is used in this study.

Restricting our attention to the in-plane mode \(k_{z} = 0\) in the 2-D photonic bandgap cavity, after some manipulations with the substitutions

\[
\mathbf{E}(x, y, z) = \mathbf{E}(x, y) \exp(-jk_{z}z),
\]

\[
\mathbf{H}(x, y, z) = \mathbf{H}(x, y) \exp(-jk_{z}z),
\]

Fig. 1. Geometry of a 2-D photonic bandgap cavity surrounded by a PML.
we can reduce Eqs. (1) to
\[
\frac{\partial}{\partial x} \left( \frac{1}{\mu_{yy}} \frac{\partial E_z}{\partial x} \right) - \frac{\partial}{\partial y} \left( \frac{1}{\mu_{xx}} \frac{\partial E_z}{\partial y} \right) - \varepsilon_{z\omega^2} E_z = 0, \quad (3)
\]
\[
\frac{\partial}{\partial x} \left( \frac{1}{\varepsilon_{yy}} \frac{\partial H_z}{\partial x} \right) - \frac{\partial}{\partial y} \left( \frac{1}{\varepsilon_{xx}} \frac{\partial H_z}{\partial y} \right) - \mu_{z\omega^2} H_z = 0. \quad (4)
\]
According to the variational principle,\textsuperscript{27} we can solve Eq. (3) by imposing the stationary requirement that \( \delta F(E_z) = 0 \) on the functional \( F(E_z) \), given by
\[
F(E_z) = \frac{1}{2} \int_{\Omega_{\text{in}}} \left[ \alpha_x \left( \frac{\partial E_z}{\partial x} \right)^2 + \alpha_y \left( \frac{\partial E_z}{\partial y} \right)^2 + \beta_z E_z^2 \right] d\Omega,
\]
where \( \alpha_x = 1/\mu_{yy} \), \( \alpha_y = 1/\mu_{xx} \), and \( \beta_z = -\varepsilon_{z\omega^2} \). The magnetic field \( H_z \) can also be determined from the same procedure described because Eqs. (3) and (4) have the same form. The functional \( F(E_z) \) cannot be evaluated by the standard finite-element discretization procedure because the infinitely extended domain of integration (\( \Omega^\text{in} \)) corresponds to an infinite number of elements. Dividing the infinite region into an interior finite-element domain \( \Omega \) and an exterior infinite region \( \Omega^\text{ext} \) by the artificial boundary \( \Gamma \) as shown in Fig. 1, we rewrite the functional for the electric field \( F(E_z) \) from Green's theorem as
\[
F(E_z) = \frac{1}{2} \int_{\Omega_{\text{in}}} \left[ \alpha_x \left( \frac{\partial E_z}{\partial x} \right)^2 + \alpha_y \left( \frac{\partial E_z}{\partial y} \right)^2 + \beta_z E_z^2 \right] d\Omega
- \frac{1}{2} \int_{\Omega_{\text{int}}} E_z \left( \alpha_x \frac{\partial E_z}{\partial x} \hat{\mathbf{x}} + \alpha_y \frac{\partial E_z}{\partial y} \hat{\mathbf{y}} \right) \cdot \hat{n} d\Gamma,
\]
(6)
where \( \hat{n} \) is the unit normal vector on the boundary \( \Gamma \) in Fig. 1. Because the electric field and the magnetic field are decoupled in the functional for the in-plane mode, it is sufficient to formulate the procedure for the TM mode solutions. The boundary integral term
\[
F_b = \frac{1}{2} \int_{\Gamma} E_z \left( \alpha_x \frac{\partial E_z}{\partial x} \hat{\mathbf{x}} + \alpha_y \frac{\partial E_z}{\partial y} \hat{\mathbf{y}} \right) \cdot \hat{n} d\Gamma
\]
(7)
in Eq. (6) must be considered carefully for open-boundary problems, and several methods have been proposed and applied for this purpose.\textsuperscript{31,32}

The anisotropic PML ABC, introduced recently by Sacks et al.,\textsuperscript{28} is employed in this study because the PML method is known to produce orders-of-magnitude smaller artificial reflectance than any earlier ABC's for the FDTD.\textsuperscript{25} According to Ref. 26, the PML layer is modeled as a nonphysical lossy anisotropic material backed with a perfect electric conductor. The elements in Eqs. (2) satisfy the conditions
\[
\epsilon_{xx} = \mu_{xx} = \frac{1}{\alpha - j\beta(x)},
\]
\[
\epsilon_{yy} = \mu_{yy} = \epsilon_{zz} = \mu_{zz} = \alpha - j\beta(x)
\]
(8)
in the PML region where the interface planes are normal to the \( y \) direction. The tangential components of the electric fields vanish on a perfect electric conductor, so the surface integral term \( F_b \) is reduced to zero by the PML method.

In the FEM the domain to be computed is subdivided into small discrete elements, the so-called finite elements. The electric field \( E_z \) and the magnetic field \( H_z \) are determined at the nodes of these elements. Dividing domain \( \Omega \) into a number of finite elements \( \Omega_e \) expands the approximate solution \( E_z^e \) in an element \( \Omega_e \) as
\[ E_z^h(x, y) = \sum_{i=1}^{n} N_i^e(x, y)E_{z,i}, \]  

(12)

where \( N_i^e(x, y) \) is the basis function for node \( i \) within element \( e \) and \( E_{z,i} \) is the complex value that corresponds to node \( i \). Substituting Eq. (12) into Eq. (6), taking \( \delta \mathbf{P} = 0 \), we obtain a generalized eigenmatrix equation:

\[ [A][E_z] - \omega^2[B][E_z] = [0], \]  

(13)

where the components of the vector \([E_z]\) are the values of \( E_z \) at nodal points, \([0]\) is a null vector, and \([A]\) and \([B]\) are global system matrices assembled from their corresponding elemental matrices given by

\[
A_{ij}^e = \int_{\Omega_e} \left( \frac{1}{\mu_y(x, y)} \frac{\partial N_i^e}{\partial x} \frac{\partial N_j^e}{\partial x} \right) \, dx, \]

(14)

\[
B_{ij}^e = \int_{\Omega_e} \varepsilon(x, y) N_i^e N_j^e \, dx. \]  

(15)

An eigenmatrix equation for TE modes is also obtained in the same manner. After solving the eigenvalue problem [Eq. (13)] we can obtain the complex eigenvalue \( \omega = \omega_r + i\omega_i \), from which the resonant frequency \( f_r = \omega_r/2\pi \) and the quality factor \( Q = \omega_i/2\omega_r \) are determined. Eigenvector \([E_z]\) corresponds to the field distribution of the resonant mode of the cavity.

**B. Higher-Order Elements and Numerical Errors**

Once a method has been established, its accuracy and efficiency must be verified. They are commonly studied by taking appropriate elements with a proper mesh that discretizes the computational domain in the FEM. Here we use linear rectangular elements and quadratic or second-order-serendipity rectangular elements and calculate the numerical errors for each case. The quadratic-serendipity rectangular element has eight nodes, as shown in Fig. 3(b). Within the element, the unknown field \( E_z \) is expressed as a quadratic function:

\[ E_z^h(x, y) = \sum_{j+k=3} a_{j,k} x^j y^k \quad (j + k \leq 3, \quad j, k \leq 2), \]  

(16)

whose eight coefficients \( a_{j,k} \) can be determined by the value of the field at the nodes. After some manipulations, Eq. (16) can be written in the form of Eq. (12) with eight basis or interpolation functions.

The error that is due to the staircase approximation can be greatly reduced by use of boundary-fitted grids that conform to the shape of physical boundaries. The FEM can treat arbitrary boundary shapes such as circular rods with higher-order elements. For example, the rounded edges that usually appear in photonic bandgap structures can be represented by quadratic elements, as shown in Fig. 4. This is an advantage of the FEM compared with other methods including the FDTD algorithm that are based primarily on an orthogonal, uniform lattice grid. In addition, the same higher-order polynomial basis functions are used to approximate fields within the corresponding element to reduce the error from the numerical dispersion, which we discuss below.

The other source of error, numerical dispersion, originates from discretization of continuous space by numerical meshes. The numerical mesh turns free space into a slightly dispersive medium. This error can be reduced by use of a finer mesh, higher-order elements to interpolate better the fields between nodes, or both. In general, the error that is due to numerical dispersion is asymptotically proportional to \( N^{-2n} \), where \( N \) denotes the number of unknowns and \( n \) denotes the order of the elements. In most wave problems an average dispersion error of less than 1% is achieved with a sampling or nodal density of 15 nodes (7 elements) per wavelength with quadratic elements, in contrast to 70 nodes per wavelength with linear elements. Although the linear element is not so good as the higher-order elements in reducing the numerical dispersion, it performs acceptably in reducing the staircase approximation error. For the design of a laser structure, better accuracy is needed for locating a resonant frequency near the peak in a gain curve properly. If one wanted to reduce errors further, the higher-order element could be used at a relatively small cost.

**C. Near-to-Far-Field Transformation**

The far-field pattern of a resonant mode is commonly measured experimentally. The field around a cavity of the resonant mode can be used to yield the far-field pattern of that resonant mode. In two dimensions the electric field for a TM mode can be obtained by Green’s theorem:

\[ \Phi_{xy} = \int_{\Omega_e} \frac{\partial \varepsilon}{\partial x} N_i^e N_j^e \mathbf{d}x. \]  

(17)

\[ \Phi_{xy} = \int_{\Omega_e} \frac{\partial \varepsilon}{\partial x} N_i^e N_j^e \mathbf{d}x. \]  

(17)
\[ E_z(r) = \oint_{C_a} [G(r|r') \hat{n}_a' \cdot \nabla E_z(r')] \\
- E_z(r') \hat{n}_a' \cdot \nabla \mathcal{G}(r|r')] \, \text{d}C', \tag{17} \]

where \( r \) is an observation point in the far-field region, \( r' \) is a source point, \( C_a \) is an arbitrary contour that encloses the arbitrary structure of interest, and \( \hat{n}_a \) is the unit outward normal vector on the contour.

In Eq. (17) the source of the field is assumed to be located within a finite region. The analytical form of the Green’s function in two dimensions, \( G(r|r') \), is given by the Hankel function expression

\[ G(r|r') = \frac{j}{4} H_0^{(2)}(k|r - r'|). \tag{18} \]

In the far-field region, \( E_z \) is given by

\[
\lim_{k|r-r'| \to \infty} E_z(r) = \frac{\exp(j3\pi/4)}{\sqrt{8\pi kr}} \exp(-jkr) \oint_{C_a} \left[ \hat{n}_a' \cdot \nabla E_z(r') - jkE_z(r') \hat{n}_a' \cdot \hat{r} \right] \\
\times \exp(jk\hat{r} \cdot r') \, \text{d}C'. \tag{19} \]

Now the radiated energy can easily be obtained from this result. The angular distribution of the far-field is expressed by the normalized radar cross section (NRCS):

\[
\text{NRCS}(\theta) = \lim_{r \to \infty} \frac{|E_z(r_\theta)|^2}{|E_z(r_c)|^2} = \frac{\oint_{C_a} \left[ \hat{n}_a' \cdot \nabla E_z(r') - jkE_z(r') \hat{n}_a' \cdot \hat{r} \right] \exp(jk\hat{r} \cdot r') \, \text{d}C'}{\oint_{C_a} \left[ \hat{n}_a' \cdot \nabla E_z(r') - jkE_z(r') \hat{n}_a' \cdot \hat{x} \right] \exp(jk\hat{x} \cdot r') \, \text{d}C'}. \tag{20} \]

Notice that NRCS becomes unity along the \( x \) axis (\( \theta = 0 \)).

3. NUMERICAL RESULTS

Our method is applied to the 2-D photonic bandgap cavity based on a square lattice with dielectric rods shown in Fig. 1. Refractive index \( n \) and the radius of the dielectric rods are 3.4 and 0.2\( a \), respectively, where \( a \) is a lattice constant. Our results are compared with those of the supercell method and the FDTD method when necessary. The photonic bandgap of the square lattice is known to be large for TM polarization. For a finite-sized cavity the \( n \times n \) notation is used to represent the size of cavity; \( n \) is the number of rods for the \( x \) axis, and we locate one defect at the center of the cavity by removing one rod.

The stability of the FEM with the PML boundary condition is tested with a \( 5 \times 5 \) cavity as we vary the number of divisions per wavelength. A parabolic absorption function \( (m = 2) \) from Eq. (9) is used in the PML. The normal reflection coefficient \( R \) of this PML is \( 1 \times 10^{-6} \). The field pattern of the resonant mode, the resonant frequency, and the \( Q \) factor are discussed. The effect of the PML parameters on the computed results are considered, and then the \( Q \) factors and the far-field patterns of the resonant mode of the \( n \times n \) cavity are calculated with the appropriate parameters.

A. Resonant Mode

The eigenvector obtained by solution of the finite-element formulation of Eq. (13) corresponds to the field pattern of a resonant mode of a \( 5 \times 5 \) cavity. The fundamental resonant mode for the cavity is plotted in Fig. 5(a) by thin and by dotted curves. Here the maximum amplitude of the \( E_z \) field is normalized to 1, and \( \log|E_z| \) is plotted. The region outside the dotted box is filled with a PML material to absorb waves from the cavity. The amplitude of the field is maximum at the center of the cavity. The amplitude of the field decreases rapidly from the center, and the energy stored in the cavity is lost along the horizontal and vertical directions. In the air region between the cavity and the PML the field spreads out because of diffraction. The amplitude of the field is nearly constant, which is typical for a traveling wave and means that the amplitude of the reflected wave is small enough not to form any noticeable interference pattern. In the PML region the amplitude of the field decreases exponentially.

The real and the imaginary parts of the field \( E_z \) at \( y = 0 \) are plotted in Fig. 5(b). A scalar factor is multiplied by field \( E_z \) to normalize the amplitude of the field and to make the imaginary part of the field zero at the center of the cavity. The imaginary part of the field is negligible near the defect and starts to appear near the outermost rods. This result implies that a standing wave is formed near the defect, and the transition from a standing wave to a traveling wave begins near the outermost rods. The real and the imaginary parts of the field have some phase difference outside the cavity, which clearly shows that traveling waves are formed outside the cavity and that they carry the stored energy in the cavity to free space. In this case the imposition of an appropriate ABC is important to minimize the nonphysical reflections of waves from the boundary of the computational domain, which is one of the major motivations of our introduction of the PML concept. Inasmuch as the traveling wave is absorbed extremely well by the PML, we can reduce the distance between the cavity and the PML to make the computational domain small. In the supercell method the calculated field pattern represents pure standing waves, and the effect of the traveling wave related to free space cannot, in principle, be included.

B. Convergence of the Method

To examine the convergence of this approach, we calculate the resonant frequency and the \( Q \) factor of the \( 5 \times 5 \) cavity as we increase the nodal density. The nodal...
density is chosen as a scalar in our analyses because the nodal density determines the size of memory needed for computation. The finer division is used in the region of the higher-refractive-index material to maintain the average number of divisions (or elements per wavelength) for the computational domain. Figure 6(a) shows that the normalized error in the resonant frequency approaches zero. It does so more rapidly with the quadratic elements. For this calculation a PML with thickness $d \sim 3\lambda_0/4$ is placed a distance $r \sim \lambda_0/2$ from the boundary of the $5 \times 5$ cavity; $\lambda_0$ denotes the reference wavelength ($\lambda_0 = 1/f_0$), which is regarded as the exact value of the resonant mode wavelength for the $5 \times 5$ cavity.

Inasmuch as the normalized error in the resonant frequency becomes extremely small at the high nodal density with the quadratic elements, we chose the value of the resonant frequency obtained at a nodal density of 42.6 as the reference ($f_0 = \omega a/2\pi c$), which is 0.37844. By studying the convergence characteristics we confirmed that the asymptotic value of the resonant frequency obtainable at the infinite nodal density cannot differ much from this reference frequency. We observed that for sufficiently small $\delta x$ (high nodal density) the error in the resonant frequency is proportional to $(\delta x)^2$ with the linear rectangular elements. In this case we reduce the error from the staircase approximation by introducing the boundary-fitted grid. Moreover, the variation of each resonant frequency stays within 0.002% of its value for various PML parameters. Then numerical dispersion becomes the main source of error. In the quadratic elements we can observe that the error in the resonant frequency is proportional to $(\delta x)^4$ and decreases even faster and independently of the PML parameters for sufficiently small $\delta x$. In addition, circular boundaries can be described exactly by the second-order polynomials with quadratic elements, which means that an overall numerical error can be estimated reliably from knowledge of the nodal density. The quadratic elements improve the convergence of resonant frequencies much better than the linear elements do. We also confirmed that our results for resonant frequency compare well with those of the supercell method using 16000 plane waves for strongly localized states.

The $Q$ factor at reference frequency $f_0$ with a nodal density of 42.6 is selected as the reference $Q$ factor $Q_0$ in Fig. 6(b). The dependence of the $Q$ factor on the PML condition is discussed in Subsection 3.C. As in the resonant frequency, the numerical dispersion is the dominant source of error in the $Q$ factor for sufficiently small $\delta x$. In one-dimensional Fabry–Perot resonators the numerical dispersion error is canceled out in the calculation of the $Q$ factor, and the $Q$ factor converges fast. However, in 2-D problems the numerical dispersion error is not canceled out in the calculation of the $Q$ factor because the amount of the numerical dispersion depends on the propagation angle. In this study we found that the convergence of the $Q$ factor seems slower than the conver-
gence of the resonant frequency. This behavior can be seen clearly if we compare the convergence of the resonant frequency and the $Q$ factor computed with the linear elements. We believe that the resonant frequency is determined mostly by the geometry near the defect. The numerical dispersion error in the resonant frequency becomes relatively insensitive to the total size of the cavity because the error is accumulated mainly in proximity to the effective cavity. However, the $Q$ factor, which contains information on the energy loss to free space, is determined by the whole cavity structure. Therefore the accuracy of the $Q$ factor depends sensitively on the numerical dispersion. Generally the error in the $Q$ factor tends to decrease as one increases the nodal density. The $Q$ factor converges much faster with the quadratic elements than with the linear elements.

C. Effect of the Perfectly Matched Layer Boundary Condition

We tested the performance of the PML by changing the PML thickness, the number of division in the PML, the order of the polynomial in the absorption function, and the normal reflection coefficient $R$. The main reason for introducing the PML is to minimize the nonphysical reflection from the boundary of the computational domain. Therefore we concentrate on the appearance of the reflected waves. We find that, using a suitable PML, the numerical errors from the reflected wave can be reduced to a desired level. First we vary the distance $r$ between the cavity and the PML to examine the effect on the results of the wave reflection at the PML. The normal reflection coefficient is set at $R = 1 \times 10^{-5}$ for all the PML’s (Fig. 7). The nodal densities with the linear and the quadratic elements are 25.2 and 19.4, respectively. The number of layers denoted in parentheses in Fig. 7 is related to the thickness of the PML for each nodal density. In fact, in Fig. 7, thirteen layers for the linear elements and five layers for the quadratic elements correspond to $\sim \lambda_0/2$ of the PML. Seventeen layers for the linear elements and eight layers for the quadratic elements correspond to $\sim 3\lambda_0/4$ of the PML. We find that the normalized resonant frequency stays constant within 0.002% in all cases, whereas the $Q$ factor oscillates as a function of the distance $r$. The period of oscillation is $\sim \lambda/2$. A similar phenomenon occurs if the distance between a weak external cavity and a Fabry–Perot resonator is varied; this means that there is a small amount of feedback of the reflected light from the PML layers to the cavity. Regardless of the PML thickness, there should be no reflection at the ideal PML. However, a small part of the incident wave is reflected at the PML because of the discretization of the domain. As the thickness of the PML is increased for a fixed value of normal reflectance $R$, the oscillating amplitude of the $Q$ factor is reduced. Therefore one can determine and place a finite-thickness PML close to the cavity without loss of computational accuracy, which is advantageous in reducing the size of computational domains.

We also varied other parameters of the PML to investigate their effects. The performance of the PML seems to be insensitive to the choice of $R$ when $R$ is smaller than $1 \times 10^{-5}$. For a fixed value of $R$ and a given number of elements dividing the PML, the $Q$ factor with a thin PML fluctuates more than that with a moderately thick PML. We also found that the amount of reflected wave decreases as one increases either the thickness or the number of divisions in the PML unless the PML is too thin. The parabolic absorption function is employed to represent the PML and is found to be reliable.

D. $n \times n$ Cavity

The resonant frequency relative to the size of the cavity is plotted in Fig. 8. The average nodal density is 19.4 with the quadratic elements. Figure 8(a) shows that the resonant frequency tends to decrease very slightly (0.1%) as the cavity size increases. This slight decrease is larger than the error limit of our calculations. The errors in convergence are less than 0.01%, and the variation of the frequencies for different PML boundary conditions is less than 0.002%.

The calculated values of the $Q$ factor relative to the size of cavity are plotted in Fig. 8(b). The $Q$ factor increases exponentially without saturation as the size increases. In this figure the $Q$ factor agrees well with results of the FDTD method. The field distribution in the inner part of the small cavity is similar to that in the large cavity, except near the outermost layers in which the boundary effect is important. The amplitude of the field decreases exponentially from the center of the cavity. As the reduction of the amplitude is related to the $Q$ factor, these observations are consistent with the exponential increase of the $Q$ factor. No resonant mode is observed for the $3 \times 3$ cavity in our program.

E. Far-Field Pattern

We studied far-field patterns because they are experimentally observable quantities. One obtains the far-field patterns of resonant modes by directly transforming the near field in the air region between the cavity and the PML. The far fields for $5 \times 5$ and $11 \times 11$ cavities are plotted in Fig. 9, which shows that the radiation is directed mostly along the two main axes. This directivity can be also observed from the field pattern of the resonant mode in Fig. 5(a). As the size of the cavity increases, the

![Fig. 7. Normalized error in the quality factor versus the distance between the structure and the PML for the different thickness of the PML. The number of layers used for the PML is denoted in parentheses. $m = 2, R = 1 \times 10^{-5}$.

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radiation along the diagonal direction is reduced. The far-field angle turns out to be almost independent of the size of the cavity.

The field pattern of the resonant mode near the defect calculated by the supercell method is almost the same as our result, but it differs from ours near the boundary of the cavity. To estimate the effect of boundary conditions we transformed the near field obtained from the supercell method to get the far-field pattern and compared the result with that from our method. Remember that the far-field pattern corresponds to the diffraction pattern of the field near the boundary. We found that the far-field pattern is totally different from ours for the $5 \times 5$ size supercell. As the size of the supercell increases, the directivity of radiation along the two main axes becomes similar to our result. However, the far-field angle is reduced in the supercell method, whereas the far-field angle is almost independent of the size of the cavity with the PML method.

4. CONCLUSION

To compute the resonant mode of the photonic bandgap cavity more rigorously we developed an eigenvalue formalism of the FEM with an anisotropic PML. Because use of the PML is a proper way to describe infinite free space, it imposes no limitation on studying cavities embedded in free space. The FEM with the higher-order elements and the PML boundary condition is an efficient way in which the resonant frequencies, the $Q$ factors, and the field pattern of the resonant mode are calculated accurately under the same conditions. The FEM with the quadratic elements is superior in convergence characteristics to that with the linear elements because of the fast reduction of the staircase approximation and of numerical dispersion errors. In our approach, various numerical errors can be reduced to below a desired level separately and systematically. The error from the reflection at the PML can be reduced by use of a thicker PML. Therefore the distance between the cavity and the PML can be decreased with a thicker PML to reduce computational domain with minimal penalty. The results computed for the resonant frequencies and the $Q$ factors are consistent with those computed by the supercell method and the FDTD method, respectively. In addition, we obtained the far-field pattern of the resonant mode directly by transforming the field in the air region surrounding the cavity. In this region the resonant mode is much different from that of the supercell method.

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REFERENCES


