Numerical Study of Three-Dimensional Photonic Crystals with Large Band Gaps

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The study presents a finite difference formulation for efficiently computing band structures of three-dimensional photonic crystals. First of all, we will show how to correctly discretize the double-curl equation for the magnetic field so that the transversality condition is exactly satisfied in the discrete sense. The first few branches of nontrivial eigenfrequencies that determine the major full band gaps of photonic crystals are computed by interlacing an inverse method with conjugate gradient projection and full multigrid acceleration. The presently developed method is applied to compute band structures of photonic crystals with modified simple cubic lattice, tetragonal square spiral structure (direct and inverse structures), and diamond structure with sp^3-like configuration. The computed results for the modified simple cubic and square spiral structures are in close agreement with those obtained by previous authors. Moreover, the sp^3-like configuration made of silicon and air is reported to have a large band gap which is larger than the largest reported elsewhere in the literature.

1. Introduction

In recent years, photonic crystals have received extensive studies because of their academic and practical interests. The most attractive/distinguished feature of photonic crystals is their full band gap structures.[1,2] Large full band gaps allow strong photon localization with the gap,[3,4] and a detailed manipulation of photonic defect states.[5,6] They have important applications such as defect cavities,[7] optical waveguides,[8] defect-mode photonic crystal lasers,[9] and feedback mirror in laser diodes.[10]

Photonic crystals, also named photonic band-gap materials, are electromagnetic analogy of electronic structures in quantum mechanics. But there are different difficulties with eigenvalue problems of the two analogous fields. It has been a challenging work to compute efficiently band structures of three-dimensional photonic crystals. In computing band structures of three-dimensional photonic crystals, we are faced with a vector (double-curl) eigenvalue problem, say, in $\boldsymbol{H}$ field formulation,

$$\nabla \times \frac{1}{\varepsilon} \nabla \times \boldsymbol{H} = \left(\frac{\omega}{c}\right)^2 \boldsymbol{H}. \tag{1}$$

It is a nontrivial problem to formulate a numerical method so that the transversality condition $\nabla \cdot \boldsymbol{H} = 0$ is correctly enforced.[11] The transversality condition can be easily done in the widely used method of plane wave expansions (PWE) by choosing, for each component $\boldsymbol{h}_G e^{i(k+G)\cdot r}$ two orthogonal polarizations $\boldsymbol{h}_G$ so that $(\boldsymbol{k}+\boldsymbol{G}) \cdot \boldsymbol{h}_G = 0$.[12] In the finite element method (FEM), the so-called vector edge elements with each individual basis function satisfying the transversality condition have been proposed for different shapes of elements.[13] Nonfulfillment of the transversality condition would lead to nonphysical spurious solutions.[14] On the other hand, finite difference is the most straightforward method to discretize the double-curl equation and the resultant matrix

is compact. For a comparison, the finite difference method (FDM) leads to a sparse matrix and ordinary matrix eigenvalue problem, whilst PWE leads to ordinary matrix problem but the matrix is always full, and FEM leads to sparse matrices, yielding a generalized eigenvalue problem. The latter statement is true of other formulations of finite element methods.[15] There are several other methods using different analytic/discrete formulations of Maxwell's equations, such as transfer matrix method,[16,17] multiple scattering method[18] and finite-difference time-domain (FDTD) method.[19,20] These different methods lead to different complexities to computing photonic band structures. However, finite difference analysis of photonic band structures in three dimensions based on direct discretization of the vector eigenvalue problem (1) has not been established in the literature.

In the present study, three important issues are addressed for the finite difference method. (i) First of all, the FDM does not use series-expansion (like PWE) nor uses any basis functions (like FEM). It is therefore essentially important that how the formulation fulfills the transversality condition. *Actually, from eq. (1), $\nabla \cdot \boldsymbol{H} = 0$ implies that the left hand side of eq. (1) must be correctly discretized so that the resultant matrix is divergence-free in the discrete sense.* (ii) If FDM is correctly formulated, the next issue of importance is the appearance of many zero eigenfrequencies, as already noted in the literature of finite element analysis.[21] The number of zero eigenfrequencies was found to be equal to the number of internal nodes of finite elements.[22] In the present finite difference formulation, it is shown to be exactly equal to the number of grid points. If the size of the matrix for the eigenvalue problem is large, it is impractical to apply a direct eigenvalue solver (such as QR algorithm[23]) or to deflate the many zeros in an iterative method (such as inverse iteration). In the study of photonic band gaps, the first few branches of non-zero eigenfrequency are of primary interest. It is therefore important that the first few non-zero frequency bands can be computed without the necessity of deflating the zero frequencies. This can be achieved by

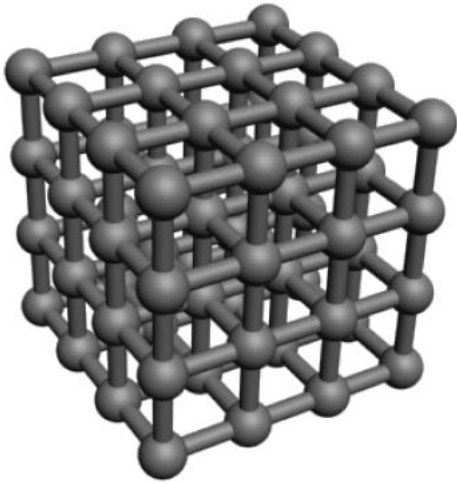*E-mail: olay@gauss.iam.ntu.edu.tw
†E-mail: changcc@gauss.iam.ntu.edu.tw

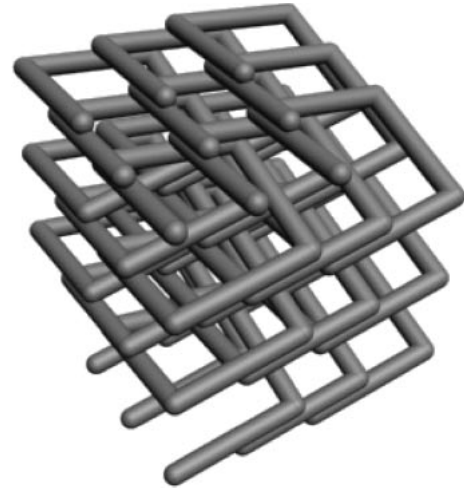Fig. 1.   Modified simple cubic lattice comprising dielectric spheres and connecting thin circular cylinders.[25]

Fig. 2.   Tetragonal square spiral structure comprising circular cylinders.[27,28]

employing projections onto the range space of the discrete matrix. (However, it is noted that the problem of many zeros does not occur in the PWE as in each plane wave component the number of polarizations is chosen to be the independent two rather three.) (iii) As the third issue of importance, it is of great interest to develop a fast algorithm for the eigenvalue problem. An inverse method, accelerated by multigrid technique with use of projection is proposed for this purpose. The method exploits the sparsity of the matrix for the eigenvalue problem in the finite difference formulation. Because of the above mentioned difficulties, the present method is a nontrivial extension of a similar method, recently developed by the authors[24] for computing photonic band structures in two dimensions.

In this study, we compute the band structures for three types of photonic structures. The first one is a modified simple cubic lattice consisting of dielectric spheres on the lattice sites, each connected to its six nearest neighbors by thin circular cylinders, which was proposed by Biswas et al.[25] Figure 1 shows the modified simple cubic lattice. It is noted that the original simple cubic structure comprising a lattice of rods has been fabricated recently with advanced silicon processing techniques.[26] The second one is the tetragonal square spiral structure comprising a lattice of circular or square cylinders, which was proposed by Toader and John,[27,28] as shown in Fig. 2. Spiral structure was discussed previously by Chutinan and Noda.[29] The square spiral structure is arranged to connect the lattice points of diamond structure with specific order, and is amenable to the current technique of fabrication GLAD (GLancing Angle Deposition) as discussed in refs. 30 and 31. As a third example, we propose a diamond structure that has sp^3-like configuration, composed of dielectric spheres with connecting spheroids, as shown in Fig. 3. Diamond structures are known to have large band gaps between relatively lower branches either in diamond network or inverse diamond structure.[12,28] In the present study, the spheroids, instead of circular cylinders, take the positions of "valence bonds" to imitate the sp^3 structure of the electrons of diamond atoms. Recently, submicron diamond-lattice photonic crystals have been successfully produced by two-photon laser nanofabri-
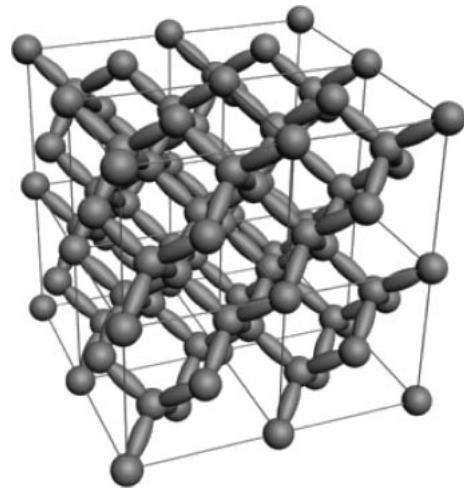

Fig. 3.   diamond structure with sp^3-like configuration comprising dielectric spheres and connecting spheroids.

cation (photopolymerization).[32]

The order of presentation of the paper is organized as follows. In §2, we show how to correctly formulate the finite difference method for the double curl operator of the photonic eigenvalue problem. In §3, we develop the numerical method (inverse iteration with the full multigrid acceleration) and present the fast algorithm, in which two alternative methods of projection are proposed to avoid the necessity of deflating zeros). In §4, we first present numerical results that illustrate the efficiency of the presently developed method. Then, the band structures are computed for the modified simple cubic lattice, the tetragonal square spiral structure (direct and inverse structure) and the diamond structure with sp^3-like configuration. Finally, concluding remarks with a summary of results are drawn in §5.

2.   Basic Equations and Finite Difference Formulation

The electromagnetic waves propagating in the photonic crystals are well described by Maxwell's equations. For linear isotropic and frequency-independent dielectric materials with permeability close to one, the time-harmonic

modes of electromagnetic waves are described by

$$LH = \left(\frac{\omega}{c}\right)^2 H \quad (2)$$

with the operator

$$L = \nabla \times \frac{1}{\varepsilon} \nabla \times \quad (3)$$

along with $\nabla \cdot H = 0$. In the above equations, $\varepsilon = \varepsilon(r)$ is the dielectric function, ω is the angular frequency of the time-harmonic modes, and c is the speed of light in vacuum. In component form, eq. (2) is written as

$$\begin{bmatrix} L_{xx} & L_{xy} & L_{xz} \\ L_{yx} & L_{yy} & L_{yz} \\ L_{zx} & L_{zy} & L_{zz} \end{bmatrix} \begin{bmatrix} H_x \\ H_y \\ H_z \end{bmatrix} = \left(\frac{\omega}{c}\right)^2 \begin{bmatrix} H_x \\ H_y \\ H_z \end{bmatrix}, \quad (4)$$

where

$$
\begin{aligned}
L_{xx} &= -\left[\frac{\partial}{\partial y}\left(\frac{1}{\varepsilon}\frac{\partial}{\partial y}\right) + \frac{\partial}{\partial z}\left(\frac{1}{\varepsilon}\frac{\partial}{\partial z}\right)\right], \\
L_{yy} &= -\left[\frac{\partial}{\partial x}\left(\frac{1}{\varepsilon}\frac{\partial}{\partial x}\right) + \frac{\partial}{\partial z}\left(\frac{1}{\varepsilon}\frac{\partial}{\partial z}\right)\right], \\
L_{zz} &= -\left[\frac{\partial}{\partial x}\left(\frac{1}{\varepsilon}\frac{\partial}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{1}{\varepsilon}\frac{\partial}{\partial y}\right)\right], \\
L_{xy} &= \frac{\partial}{\partial y}\left(\frac{1}{\varepsilon}\frac{\partial}{\partial x}\right), \quad L_{xz} = \frac{\partial}{\partial z}\left(\frac{1}{\varepsilon}\frac{\partial}{\partial x}\right), \\
L_{yx} &= \frac{\partial}{\partial x}\left(\frac{1}{\varepsilon}\frac{\partial}{\partial y}\right), \quad L_{yz} = \frac{\partial}{\partial z}\left(\frac{1}{\varepsilon}\frac{\partial}{\partial y}\right), \\
L_{zx} &= \frac{\partial}{\partial x}\left(\frac{1}{\varepsilon}\frac{\partial}{\partial z}\right), \quad L_{zy} = \frac{\partial}{\partial y}\left(\frac{1}{\varepsilon}\frac{\partial}{\partial z}\right),
\end{aligned}
\quad (5)
$$

and H_x, H_y and H_z are components of the H field.

This section is aimed to discretize the operator L on the left hand side of eq. (2) so that the transversality condition is correctly imposed in discrete sense. For this purpose, we first take the divergence of eq. (2) and integrate over a unit grid cell V_{cell}, which is shown in Fig. 4. In this figure, H_x, H_y and H_z are interleaved to occupy the sites of front and rear, left and right, top and bottom sites, respectively. The reason of choosing this becomes clear shortly. Applying the divergence theorem, we have

$$\int_{V_{\text{cell}}} \nabla \cdot (LH) d\tau = \sum_{l=1}^{6} \int_{S_l} (LH) \cdot n da, \quad (6)$$

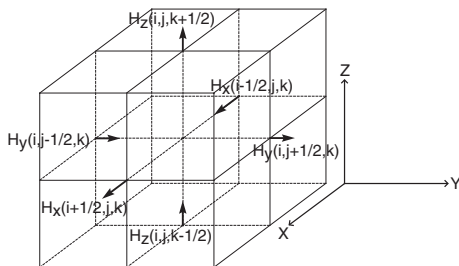where S_l, $l = 1$ to 6 are the six surfaces enclosing V_{cell}. Next,

Fig. 4. The unit grid cell for finite difference formulation. H_x, H_y and H_z are interleaved to occupy the front and rear, left and right, top and bottom sites, respectively.

we approximate the right hand side of eq. (6) by

$$0 = \sum_{l=1}^{6} \int_{S_l} (LH) \cdot n da \approx \sum_{l=1}^{6} \left(\nabla \times \frac{1}{\varepsilon} \nabla \times H\right)_{C_l} \cdot nA, \quad (7)$$

where C_l denotes the center of S_l and A is the area of S_l. Now we approximate the double-curl operator on the right hand side of eq. (7) at the centers C_l of six surfaces S_l by a second-order central difference scheme. For example, consider $L_{xx}H_x$ and $L_{xy}H_y$ at the center of front surface of V_{cell}. First, the first-order derivatives at the middle points $(i + 1/2, j + 1/2, k)$ of the H field are approximated by

$$\left(\frac{\partial H_x}{\partial y}\right)_{i+1/2,j+1/2,k} \approx \frac{1}{h}\left((H_x)_{i+1/2,j+1,k} - (H_x)_{i+1/2,j,k}\right), \quad (8)$$

where h is the grid spacing. Then the second-order derivatives are approximated using the above derivatives,

$$
\begin{aligned}
&\frac{\partial}{\partial y}\left(\frac{1}{\varepsilon}\frac{\partial H_x}{\partial y}\right)_{i+1/2,j,k} \\
&\approx \frac{1}{h}\left(\left(\frac{1}{\varepsilon}\frac{\partial H_x}{\partial y}\right)_{i+1/2,j+1/2,k} - \left(\frac{1}{\varepsilon}\frac{\partial H_x}{\partial y}\right)_{i+1/2,j-1/2,k}\right).
\end{aligned}
\quad (9)
$$

Substituting (8) for the derivatives in (9) eliminates the middle fields at $(i + 1/2, j \pm 1/2, k)$. The complete finite difference formulation for the diagonal term $L_{xx}H_x$ is

$$
\begin{aligned}
(L_{xx}&H_x)_{i+1/2,j,k} \\
&\approx \frac{1}{h^2}\left(\frac{H_x^{i+1/2,j,k}}{\varepsilon_{i+1/2,j-1/2,k}} + \frac{H_x^{i+1/2,j,k}}{\varepsilon_{i+1/2,j+1/2,k}}\right) \\
&+ \frac{1}{h^2}\left(\frac{H_x^{i+1/2,j,k}}{\varepsilon_{i+1/2,j,k-1/2}} + \frac{H_x^{i+1/2,j,k}}{\varepsilon_{i+1/2,j,k+1/2}}\right) \\
&- \frac{1}{h^2}\left(\frac{H_x^{i+1/2,j-1,k}}{\varepsilon_{i+1/2,j-1/2,k}} + \frac{H_x^{i+1/2,j+1,k}}{\varepsilon_{i+1/2,j+1/2,k}}\right) \\
&- \frac{1}{h^2}\left(\frac{H_x^{i+1/2,j,k-1}}{\varepsilon_{i+1/2,j,k-1/2}} + \frac{H_x^{i+1/2,j,k+1}}{\varepsilon_{i+1/2,j,k+1/2}}\right)
\end{aligned}
\quad (10)
$$

and the off-diagonal term $L_{xy}H_y$ is

$$
\begin{aligned}
\left(L_{xy}H_y\right)_{i+1/2,j,k} &\approx \frac{1}{h^2}\left(\frac{H_y^{i,j-1/2,k}}{\varepsilon_{i+1/2,j-1/2,k}} - \frac{H_y^{i+1,j-1/2,k}}{\varepsilon_{i+1/2,j-1/2,k}}\right) \\
&- \frac{1}{h^2}\left(\frac{H_y^{i,j+1/2,k}}{\varepsilon_{i+1/2,j+1/2,k}} - \frac{H_y^{i+1,j+1/2,k}}{\varepsilon_{i+1/2,j+1/2,k}}\right). \quad (11)
\end{aligned}
$$

Likewise, we discretize the other terms in eq. (5) in a similar way, and collect the results into eq. (7). Altogether, there are 96 terms in these approximations. *The 96 terms cancel each other exactly, showing that the transversality condition is satisfied in a discrete form of eq. (6).* The discrete transversality condition is satisfied even when the grid cell cross the interface of different dielectric materials. The detailed proof of the discrete transversality condition is given in Appendix A. Indeed, our numerical experiments further confirm this condition by giving 64 zero eigenvalues for matrix of size 192×192 (grid size $4 \times 4 \times 4$), and 512 zeros for matrix of size 1536×1536 (grid size $8 \times 8 \times 8$).

It is now cleared that the grid arrangement in Fig. 4 is sufficient to fulfill the transversality condition in the present finite difference formulation. Namely, we use H_x only at half-integer points $i + 1/2$ and integer points j and k, H_y at half-integer points $j + 1/2$ and integer points i and k, and H_z

at half-integer points $k + 1/2$ and integer points i and j. For simplicity, we denote $(i + 1/2, j, k)$ by $a/2$, $(i, j + 1/2, k)$ by $b/2$ and $(i, j, k + 1/2)$ by $c/2$. To be consistent with the above finite difference formulation, the double-curl operator in eq. (3) is discretized to yield a discretization matrix A as follows:

$$[\mathbf{A}\mathbf{H}]_{i,j,k} \equiv \begin{bmatrix} L_{xx} & L_{xy} & L_{xz} \\ L_{yx} & L_{yy} & L_{yz} \\ L_{zx} & L_{zy} & L_{zz} \end{bmatrix}_{\text{C.D.}} \begin{bmatrix} H_x^{a/2} \\ H_y^{b/2} \\ H_z^{c/2} \end{bmatrix}, \quad (12)$$

where "C.D." denotes that the central difference is applied. The matrix A has 39 finite difference terms. Appendix B contains all the details. It is also noticed that the space arrangement for the H field is equivalent to that in Yee's cell,[33] but the formulation, which contains second-order derivatives, is different from Yee's scheme. In the finite element method, the vector edge elements have been proposed to satisfy the transversality condition.[13] In their formulations, the transversality condition is satisfied on each individual basis function while in the present method, the transversality condition is satisfied in a less obvious way.

If the matrix size is small, the eigenvalues can be obtained by direct methods. However, the operation count is of order N^3, which becomes prohibitively large for large N. The difficulty of large operation counts can be alleviated by an iterative solver, but the large number of zero eigenvalues causes another difficulty. Zero modes appear before any nontrivial eigenmodes when we solve the eigenfrequencies from the smallest one. Therefore, it is impractical and inaccurate to deflate a large number of zero eigenmodes. In the present study, deflation of zero modes is avoided by introducing a projection operator onto the range space of the matrix A, which will be discussed in the next section.

Next, it is very important to choose the domain of computation that is advantageous to the finite difference formulation. For the three types of configuration, the domains of computation are chosen to be; (i) a cubic coincident with the primitive cell for the modified simple cubic lattice, as shown in Fig. 5, (ii) a tetragon coincident with the primitive cell for the tetragonal square spiral
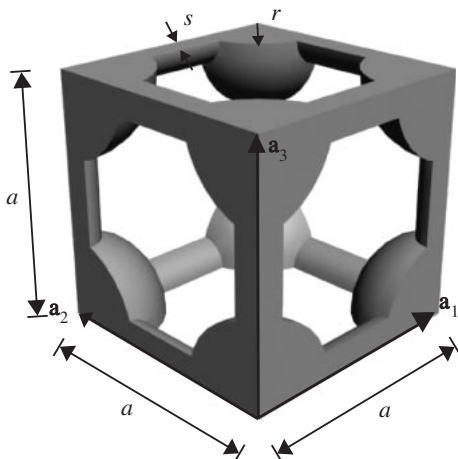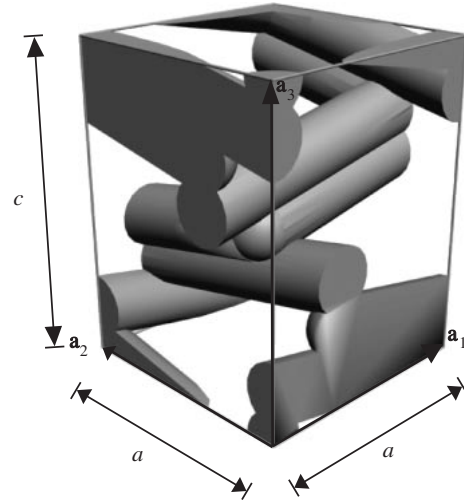

Fig. 6. Domain of computation for the tetragonal square spiral structure in Fig. 2 is a tetragon with square of side length a and height c. The square spiral structure is composed of circular cylinder with radius r, length L and pitch c.

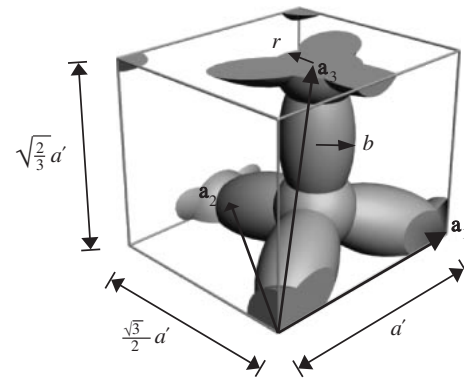Fig. 7. Domain of computation for the diamond structure with sp^3-like configuration in Fig. 3 is a tetragon with length a', width $a'\sqrt{3}/2$ and height $a'\sqrt{2/3}$, where $a' = a/\sqrt{2}$ with a the lattice constant. The radius of the dielectric sphere is r. The connecting spheroid has minor axis length b, and the foci located at the centers of the spheres.

structure, as shown in Fig. 6, and (iii) a tetragon with one edge aligned with one of the lattice translation vectors for the diamond structure with sp^3-like configuration. This domain has and must have the same volume of the primitive cell as shown in Fig. 7.

Finally, Bloch's theorem is applied at the boundary of domain of computation:

$$\mathbf{H}_k(\mathbf{r} + \mathbf{a}_i) = e^{i\mathbf{k}\cdot\mathbf{a}_i} \mathbf{H}_k(\mathbf{r}), \quad (13)$$

where $\mathbf{H}_k$ is the Bloch function for magnetic field associated with the wave vector $\mathbf{k}$ in the first Brillouin zone. The letters $\mathbf{a}_i$ $(i = 1, 2, 3)$ denote the lattice translation vectors; (i) for the modified simple cubic lattice, $\mathbf{a}_1 = a(1, 0, 0)$, $\mathbf{a}_2 = a(0, 1, 0)$ and $\mathbf{a}_3 = a(0, 0, 1)$, (ii) for the tetragonal square spiral structure, $\mathbf{a}_1 = a(1, 0, 0)$, $\mathbf{a}_2 = a(0, 1, 0)$ and $\mathbf{a}_3 = c(0, 0, 1)$, and (iii) for the diamond structure, $\mathbf{a}_1 = a'(1, 0, 0)$, $\mathbf{a}_2 = a'(1/2, \sqrt{3}/2, 0)$ and $\mathbf{a}_3 = a'(1/2, 1/2\sqrt{3}, \sqrt{2/3})$ with $a' = a/\sqrt{2}$. In the last case, since $\mathbf{a}_2$ and $\mathbf{a}_3$ have the component $a'/2$ in the x-direction, application of Bloch's theorem in the y- and z-directions should be additionally

Fig. 5. Domain of computation for the modified simple cubic lattice in Fig. 1 is a cube with side length a. The radius of the dielectric sphere is r and the radius of the connecting cylinder is s.
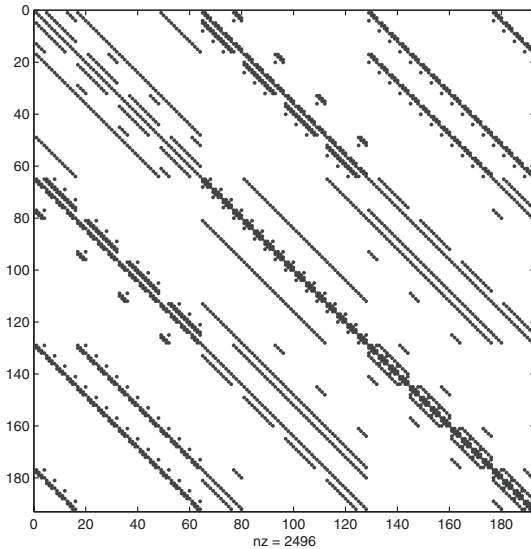
Fig. 8.   13-band structure of the discretization matrix A of size 192×192.

accompanied by the shift of one-half cell in the x-direction. Furthermore, a_3 has the component $a'/2\sqrt{3} = (a'\sqrt{3}/2)/3$ in the y-direction, application of Bloch's condition in the z-direction should be further accompanied by the shift of one-third cell in the y-direction.

3.   Inverse Method With Multigrid Acceleration and Methods of Projection

In eq. (12) we obtain the discretization matrix A of the vector differential operator L. The matrix structure is shown in Fig. 8. Matrix A has a sparsity pattern very different from that for the two-dimensional operators (either in transverse-electric or magnetic modes). For the two-dimensional case, there are only 5 nonzero entries in each row of A, but there are 13 nonzero entries in each row for the three-dimensional case. For example, the number of nonzero entries of matrix A of size 192×192 (grid size $4 \times 4 \times 4$) is $192 \times 13 = 2496$.

3.1   Inverse iteration

From a practical point of view, the first few branches of eigenvalues are of primary interest. A natural choice for this purpose is the method of inverse iteration, applied to obtain the smallest eigenvalues as well as the corresponding eigenvectors. For the eigenvalue problem

$$Ax = \lambda x, \qquad (14)$$

the method of inverse iteration finds the smallest eigenvalue, which is closest to μ, by iteratively solving

$$(A - \mu I)x = b. \qquad (15)$$

The second eigenvalue is obtained by repeating the same method with deflation of the first eigenvector. The third eigenvalue is obtained by repeating the same method with deflating the first and second eigenvectors, and so on. In particular, the Gram–Schmidt orthogonalization is used to deflate, or to eliminate the components of previously obtained eigenvectors. The inverse algorithm[23,34] is presented as follows:

```
InverseEigen {
    for n = 1 to S
        Initial guess b
        do
            Solve (A − μI)x = b by LUD or PCG
            Deflate x by q₁ to qₙ₋₁
            Set b = x/‖x‖
                Rayleigh Quotient λₙ = ⟨b, Ab⟩
        until ‖(A − λₙI)b‖₂ < ε
        Set qₙ = b
    end }
```

where μ is the parameter for inverse iteration, $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_S$ is the sequence of S smallest eigenvalues, and q_1 to q_S are the corresponding eigenvectors. The inner product $\langle \cdot, \cdot \rangle$ is defined as

$$\langle x, y \rangle = \sum_i \bar{x}_i y_i \qquad (16)$$

in view of the orthonormalization property of the H field:

$$\frac{1}{V_{\text{cell}}} \int_{V_{\text{cell}}} H_m^*(r) \cdot H_n(r) dr = \delta_{mn}, \qquad (17)$$

where H_n is the nth eigenmode of the magnetic field, V_{cell} is the volume of the primitive cell and δ_{mn} denotes the Kronecker delta. **LUD** denotes the lower–upper decomposition solver for matrix inversion, and **PCG** the preconditioned conjugate gradient solver.

3.2   Methods of projection

In §2, we mentioned that matrix A has $N/3$ zero modes, where $N = 3n^3$ for the grid size $n \times n \times n$. Since only the first few nontrivial eigenmodes are of practical interests, it is important to remove from the iterated solutions the components of the null (zero-mode) space $N(A) = \{x | Ax = 0\}$. But it would be impractical and inaccurate to delate all the $N/3$ zero modes. Instead, we propose two methods of projection onto the range space $R(A) = \{Ax\}$ that dispenses with the necessity of deflating the many zero modes.

3.2.1   Projection by multiplying A

In the original inverse algorithm, we iteratively solve

$$x = \frac{1}{(A - \mu I)} b \qquad (18)$$

to obtain the eigenvector x. Let z be any solution corresponding to zero frequency, that is, $Az = 0$. Taking inner product with x, and using the Hermitian property of A, we obtain $\langle x, Az \rangle = \langle Ax, z \rangle = 0$. The result indicates that Ax is orthogonal to z. We can therefore multiply the solution x by A to eliminate the components of zero modes z. This idea is implemented by modifying the inverse algorithm as

$$x = \frac{1}{(A - \mu I)^2} Ab. \qquad (19)$$

This is equivalent to applying a forward iteration without shift followed by two inverse iterations with shift μ. The overall effect is one inverse iteration, as is the original inverse algorithm. The new algorithm, however, removes the components of zero modes at each iteration, keeping the iterative solutions falling into the range space of A.

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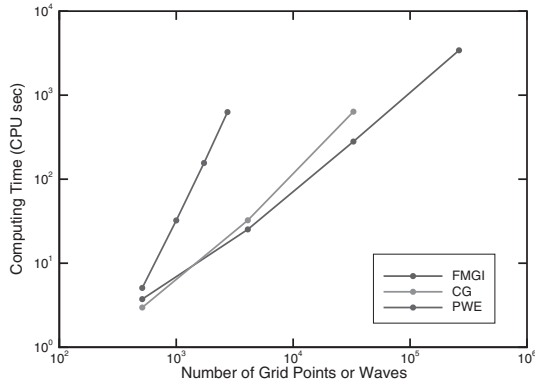Fig. 9. Comparison of the present method, conjugate gradient method and plane wave expansions in computing time.

Fig. 10. Band structure computed with $48 \times 48 \times 48$ grid for the modified simple cubic lattice in Fig. 1 at $r/a = 0.345$ and $s/a = 0.11$ for $\varepsilon/\varepsilon_0 = 13$.

Fig. 11. Band structure computed with $48 \times 48 \times 48$ grid for the tetragonal square spiral structure in Fig. 2 at $r/a = 0.13$, $c/a = 1.3$ and $L/a = 1.65$ for $\varepsilon/\varepsilon_0 = 13$.

The plot of the computing times is shown in Fig. 9. All the computations are performed on a Pentium 4-2.8 GHz PC. The computing time for the present method is of order $N^{1.18}$, which is slightly larger than order N for the two-dimensional problems.[24] This is because additional computations are due to the conjugate gradient projection, which is in general slower than the pure multigrid method. If the multigrid solver is replaced by the conjugate gradient method, the computing time is of order $N^{1.43}$. On the other hand, the direct plane wave expansion has the computational cost of about the order $N^{2.87}$. However, it must be noticed that iterative solvers with suitable preconditioners may significantly reduce the operation counts for PWE.[39]

The accuracy of the present method is illustrated by the convergence test against the grid size for the band edges and gap–midgap ratios for the optimized diamond structure with sp^3-like configuration. Computations are performed on three different grids: $N = 24 \times 24 \times 24$, $48 \times 48 \times 48$ and $96 \times 96 \times 96$. Table II lists the numerics of the location of the band edge for the diamond structure with sp^3-like configuration in Fig. 2. Basically, the computed results agree with each other to three significant digits. In other words, the relative differences of the computed results with the different grids are less than 0.1%.

Figure 10 shows the band structure for the modified simple cubic lattice in Fig. 1 at $r/a = 0.345$ and $s/a = 0.11$ for $\varepsilon/\varepsilon_0 = 13$. The complete band gap lies between the 5th and 6th branches with the lower edge located at point X and the upper edge at point M. The gap–midgap ratio is 0.1363 with center frequency 0.4501. The modified simple cubic lattice was previously investigated by Biswas *et al.*, who obtained a gap–midgap ratio 0.12 for $\varepsilon/\varepsilon_0 = 12.96$.[25] At the same geometric parameters, the overall band structure of the

present study is in reasonably good agreement with their results. However, our gap–midgap ratio is somewhat larger. One possible reason for this could be that there are relatively smaller number of plane waves used in ref. 25, compared to the presently larger number of grid points $N = 48 \times 48 \times 48$.

Figure 11 shows the band structure for the tetragonal square spiral structure in Fig. 2 at $r/a = 0.13$, $c/a = 1.3$ and $L/a = 1.65$ for $\varepsilon/\varepsilon_0 = 13$. A photonic band gap with gap–midgap ratio 0.162 opens between the 4th and 5th bands. The upper edge closes at point R and the lower edge at point A. The center frequency of the band gap is 0.3974. Figure 12 shows the band structure for the inverse structure of the tetragonal square spiral structure with $r/a = 0.333$, $c/a = 1.69$ and $L/a = 1.5$ for $\varepsilon/\varepsilon_0 = 13$. The inverse structure has a similar band structure with the band edges occurring at the same symmetric points: R (upper) and A (lower), but with an even larger band gap. The gap–midgap ratio is 0.2593 with center frequency 0.3826. These configurations were studied by Toader and John, who obtained the gap–midgap ratios 0.162 and 0.236 for direct and inverse structures, respectively, for $\varepsilon/\varepsilon_0 = 11.9$.[28] For the direct structure, their gap–midgap ratio is identical to that obtained in the present study, while for the inverse structure, our result is a little bit larger.

Figure 13 shows the band structure for the diamond structure with sp^3-like configuration in Fig. 3 at $r/a = 0.12$

Table II. Convergence test against the grid size for the band edges and gap–midgap ratios of the diamond structure with sp^3-like configuration in Fig. 3 for $r/a = 0.12$ and $b/a = 0.11$.

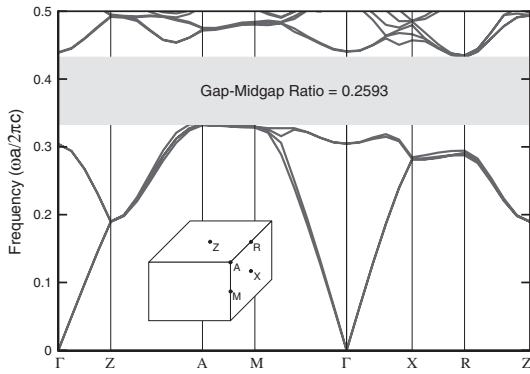| N_{grid}	$24 \times 24 \times 24$	$48 \times 48 \times 48$	$96 \times 96 \times 96$
ω_{up}	0.6890	0.6879	0.6874
ω_{low}	0.5016	0.5013	0.5010
ω_{mid}	0.5953	0.5946	0.5942
$\Delta\omega$	0.1874	0.1866	0.1864
$\Delta\omega/\omega_{mid}$	0.3147	0.3139	0.3137

Fig. 12.   Band structure computed with $48 \times 48 \times 48$ grid for the inverse structure of tetragonal square spiral at $r/a = 0.333$, $c/a = 1.69$ and $L/a = 1.5$ for $\varepsilon/\varepsilon_0 = 13$.

Fig. 14.   The effect of preconditioners on the convergence of the conjugate gradient method as an eigenvalue solver of two-dimensional photonic crystals.

Fig. 13.   Band structure computed with $48 \times 48 \times 48$ grid for the diamond structure with sp^3-like configuration in Fig. 3 at $r/a = 0.12$ and $b/a = 0.11$ for $\varepsilon/\varepsilon_0 = 13$.
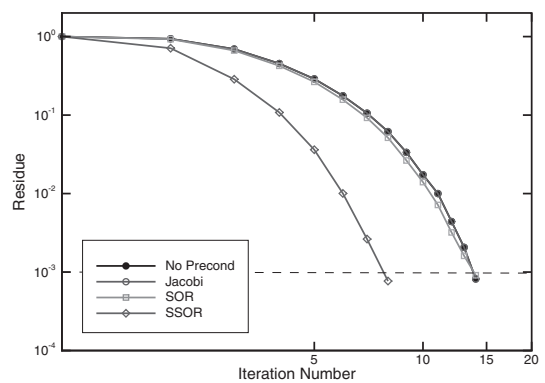
Fig. 15.   The effect of preconditioners on the convergence of the conjugate gradient method for the three-dimensional Laplace equation.
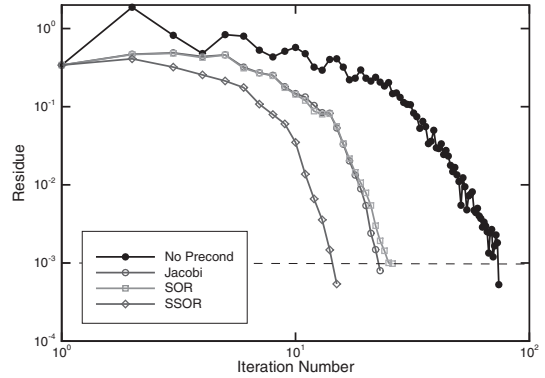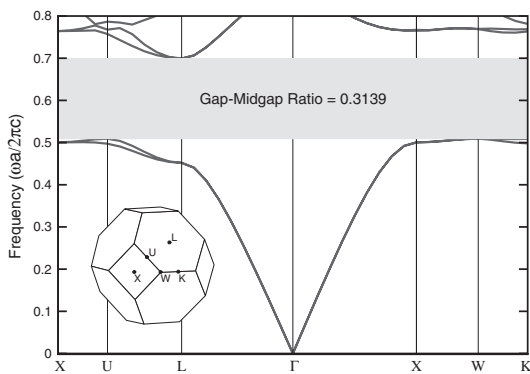

Fig. 16.   The effect of preconditioners on the convergence of the conjugate gradient method as an eigenvalue solver of three-dimensional photonic crystals.

and $b/a = 0.11$ for $\varepsilon/\varepsilon_0 = 13$. A large photonic band gap occurs between the 2nd and 3rd branches with gap–midgap ratio 0.3139 and center frequency 0.5946. This band gap has the upper edge at point L and the lower edge at point W. The lower edge from W to K is a flat curve, which almost has the edge value at point U. It is rather interesting to notice that the gap is found to be larger than ever reported in the literature for any other three-dimensional photonic crystals.

Finally, we illustrate the difficulty in accelerating convergence of numerical methods for computing three-dimensional photonic band structures. For this, we compare convergence of the conjugate gradient solver for computing two- and three-dimensional photonic band structures as well as three-dimensional Laplace equation. The conjugate gradient method is preconditioned with Jacobi, SOR or SSOR preconditioners.[38,40] For two-dimensional problem, these preconditioners do help accelerate convergence of the conjugate gradient method for the eigenvalue solver. Figure 14 shows the effect of these preconditioners on the convergence of the eigenvalue solver for the first band at point X for a square lattice. The relaxation parameter has been optimized for best convergence in each case. Figure 15 shows the effect of these preconditioners on the convergence of the three-dimensional Laplace equation. Likewise, the relaxation parameters have been optimized for best convergence. The results show that the SSOR preconditioner accelerates convergence while the other three do not

accelerate convergence. In spite of the two successful examples, none of the well-known preconditioners are effective in accelerating convergence of the conjugate gradient method as an eigenvalue solver for three-dimensional photonic crystals. Figure 16 shows the effect of these preconditioners on the first band at point X for the modified simple cubic lattice. The results show that these preconditioners do not accelerate and even slow down the convergence. There might be some other preconditioners which are suitable for the three-dimensional photonic crystals, but

they would be very much problem-dependent. On the other hand, the presently developed method are applicable to compute band structures of three-dimensional photonic crystals of arbitrary configuration with strong dielectric interfaces.

5. Conclusions

In the present study, an efficient method in finite difference formulation was developed for computing band structures of three-dimensional photonic crystals. The method is a substantial extension of our two-dimensional version. (i) First, we have shown how the transversality condition can be satisfied for the vector eigenvalue problem in the finite difference formulation. (ii) Second, fulfillment of the transversality condition results in a large number of unwanted zero-frequency modes. The number of zero frequencies is exactly equal to the number of the internal nodes. The method of inverse iteration has been applied to obtain the first few nontrivial eigenmodes. Projection by the matrix itself, or conjugate gradient method has been employed to avoid the necessity of deflating a large number of zero eigenmodes. (iii) Third, fast computation of photonic band structures is achieved by embedding inverse iteration in the full multigrid algorithm with use of the method of projection. The present method was shown to have a computational cost of order $N^{1.18}$, which is slightly larger than the linear order N for the two-dimensional problems.[24] This is due to the more expensive part of the conjugate gradient projection. Nevertheless, the method is much faster than the most commonly used method of plane wave expansions, which has been demonstrated to be of order $N^{2.87}$.

The accuracy of the present method has been tested against various grid sizes from $N = 24 \times 24 \times 24$ to $96 \times 96 \times 96$, and basically the results agree to each other to three significant digits. Examples of applications include (i) the modified simple cubic lattice, (ii) the tetragonal square spiral structure (direct and inverse structure), and (iii) the diamond structure with sp^3-like configuration. The first two examples were previously studied by other authors.[25,27,28] Our numerical results are in close agreement with those obtained by previous authors. However, with the fast algorithm the band structures presented in this study can be easily computed with the grid of size $N = 48 \times 48 \times 48$, compared to the relatively small $N = 1400$[28] used in plane wave expansions. Both the second and third examples may be considered as modifications of the diamond structure. The second example is amenable to the successful fabrication technique: GLAD (GLancing Angle Deposition). The third example with sp^3-like configuration made of silicon and air proposed by the present authors has a large band gap with gap–midgap ratio 0.3139, which is larger than ever reported in the literature. The latter result is of particular interest in view of recently successful production of diamond-lattice photonic crystals by two-photon laser nanofabrication (photopolymerization).[32] In general, our numerical experience indicates that the diamond-like structures and their modifications are the *ideal* three-dimensional configurations to produce large photonic band gaps. As a matter of fact, if square spirals are replaced by triangular or hexagonal spirals, we do not find any significant band gaps for these configurations. These examples have demonstrated that the presently developed method is capable of resolving the multieigenvalue band structures of three-dimensional photonic crystals of arbitrary configuration with strong dielectric interfaces. The method is currently being extended to be applicable to metallic and metallodielectric photonic crystals; the results will be reported elsewhere.

Appendix A: Proof of the Discrete Transversality Condition

Recall that we denote $(i + 1/2, j, k)$ by $a/2$, $(i, j + 1/2, k)$ by $b/2$ and $(i, j, k + 1/2)$ by $c/2$. The complete discretized finite difference formulation of eq. (7) can be written as

$$\sum_{l=1}^{6} \left(\nabla \times \frac{1}{\varepsilon} \nabla \times \boldsymbol{H} \right)_{C_l} \cdot \boldsymbol{n} A$$
$$= G_x^{a/2} + G_y^{b/2} + G_z^{c/2} - G_x^{-a/2} - G_y^{-b/2} - G_z^{-c/2},$$

$$G_x^{a/2}$$
$$\approx \left(\frac{H_x^{a/2}}{\varepsilon_{a/2,-b/2}} + \frac{H_x^{a/2}}{\varepsilon_{a/2,b/2}} + \frac{H_x^{a/2}}{\varepsilon_{a/2,-c/2}} + \frac{H_x^{a/2}}{\varepsilon_{a/2,c/2}} \right)$$
$$- \left(\frac{H_x^{a/2,-b}}{\varepsilon_{a/2,-b/2}} + \frac{H_x^{a/2,b}}{\varepsilon_{a/2,b/2}} + \frac{H_x^{a/2,-c}}{\varepsilon_{a/2,-c/2}} + \frac{H_x^{a/2,c}}{\varepsilon_{a/2,c/2}} \right)$$
$$+ \left(\frac{H_y^{-b/2}}{\varepsilon_{a/2,-b/2}} - \frac{H_y^{a,-b/2}}{\varepsilon_{a/2,-b/2}} - \frac{H_y^{b/2}}{\varepsilon_{a/2,b/2}} + \frac{H_y^{a,b/2}}{\varepsilon_{a/2,b/2}} \right)$$
$$+ \left(\frac{H_z^{-c/2}}{\varepsilon_{a/2,-c/2}} - \frac{H_z^{a,-c/2}}{\varepsilon_{a/2,-c/2}} - \frac{H_z^{c/2}}{\varepsilon_{a/2,c/2}} + \frac{H_z^{a,c/2}}{\varepsilon_{a/2,c/2}} \right),$$

$$G_y^{b/2}$$
$$\approx \left(\frac{H_y^{b/2}}{\varepsilon_{-a/2,b/2}} + \frac{H_y^{b/2}}{\varepsilon_{a/2,b/2}} + \frac{H_y^{b/2}}{\varepsilon_{b/2,-c/2}} + \frac{H_y^{b/2}}{\varepsilon_{b/2,c/2}} \right)$$
$$- \left(\frac{H_y^{-a,b/2}}{\varepsilon_{-a/2,b/2}} + \frac{H_y^{a,b/2}}{\varepsilon_{a/2,b/2}} + \frac{H_y^{b/2,-c}}{\varepsilon_{b/2,-c/2}} + \frac{H_y^{b/2,c}}{\varepsilon_{b/2,c/2}} \right)$$
$$+ \left(\frac{H_x^{-a/2}}{\varepsilon_{-a/2,b/2}} - \frac{H_x^{-a/2,b}}{\varepsilon_{-a/2,b/2}} - \frac{H_x^{a/2}}{\varepsilon_{a/2,b/2}} + \frac{H_x^{a/2,b}}{\varepsilon_{a/2,b/2}} \right)$$
$$+ \left(\frac{H_z^{-c/2}}{\varepsilon_{b/2,-c/2}} - \frac{H_z^{b,-c/2}}{\varepsilon_{b/2,-c/2}} - \frac{H_z^{c/2}}{\varepsilon_{b/2,c/2}} + \frac{H_z^{b,c/2}}{\varepsilon_{b/2,c/2}} \right),$$

$$G_z^{c/2}$$
$$\approx \left(\frac{H_z^{c/2}}{\varepsilon_{-a/2,c/2}} + \frac{H_z^{c/2}}{\varepsilon_{a/2,c/2}} + \frac{H_z^{c/2}}{\varepsilon_{-b/2,c/2}} + \frac{H_z^{c/2}}{\varepsilon_{b/2,c/2}} \right)$$
$$- \left(\frac{H_z^{-a,c/2}}{\varepsilon_{-a/2,c/2}} + \frac{H_z^{a,c/2}}{\varepsilon_{a/2,c/2}} + \frac{H_z^{-b,c/2}}{\varepsilon_{-b/2,c/2}} + \frac{H_z^{b,c/2}}{\varepsilon_{b/2,c/2}} \right)$$
$$+ \left(\frac{H_x^{-a/2}}{\varepsilon_{-a/2,c/2}} - \frac{H_x^{-a/2,c}}{\varepsilon_{-a/2,c/2}} - \frac{H_x^{a/2}}{\varepsilon_{a/2,c/2}} + \frac{H_x^{a/2,c}}{\varepsilon_{a/2,c/2}} \right)$$
$$+ \left(\frac{H_y^{-b/2}}{\varepsilon_{-b/2,c/2}} - \frac{H_y^{-b/2,c}}{\varepsilon_{-b/2,c/2}} - \frac{H_y^{b/2}}{\varepsilon_{b/2,c/2}} + \frac{H_y^{b/2,c}}{\varepsilon_{b/2,c/2}} \right),$$

$G_x^{-a/2}$

$$\approx \left(\frac{H_x^{-a/2}}{\varepsilon_{-a/2,-b/2}} + \frac{H_x^{-a/2}}{\varepsilon_{-a/2,b/2}} + \frac{H_x^{-a/2}}{\varepsilon_{-a/2,-c/2}} + \frac{H_x^{-a/2}}{\varepsilon_{-a/2,c/2}} \right)$$
$$- \left(\frac{H_x^{-a/2,-b}}{\varepsilon_{-a/2,-b/2}} + \frac{H_x^{-a/2,b}}{\varepsilon_{-a/2,b/2}} + \frac{H_x^{-a/2,-c}}{\varepsilon_{-a/2,-c/2}} + \frac{H_x^{-a/2,c}}{\varepsilon_{-a/2,c/2}} \right)$$
$$+ \left(\frac{H_y^{-a,-b/2}}{\varepsilon_{-a/2,-b/2}} - \frac{H_y^{-b/2}}{\varepsilon_{-a/2,-b/2}} - \frac{H_y^{-a,b/2}}{\varepsilon_{-a/2,b/2}} + \frac{H_y^{b/2}}{\varepsilon_{-a/2,b/2}} \right)$$
$$+ \left(\frac{H_z^{-a,-c/2}}{\varepsilon_{-a/2,-c/2}} - \frac{H_z^{-c/2}}{\varepsilon_{-a/2,-c/2}} - \frac{H_z^{-a,c/2}}{\varepsilon_{-a/2,c/2}} + \frac{H_z^{c/2}}{\varepsilon_{-a/2,c/2}} \right),$$

$G_y^{-b/2}$

$$\approx \left(\frac{H_y^{-b/2}}{\varepsilon_{-a/2,-b/2}} + \frac{H_y^{-b/2}}{\varepsilon_{a/2,-b/2}} + \frac{H_y^{-b/2}}{\varepsilon_{-b/2,-c/2}} + \frac{H_y^{-b/2}}{\varepsilon_{-b/2,c/2}} \right)$$
$$- \left(\frac{H_y^{-a,-b/2}}{\varepsilon_{-a/2,-b/2}} + \frac{H_y^{a,-b/2}}{\varepsilon_{a/2,-b/2}} + \frac{H_y^{-b/2,-c}}{\varepsilon_{-b/2,-c/2}} + \frac{H_y^{-b/2,c}}{\varepsilon_{-b/2,c/2}} \right)$$
$$+ \left(\frac{H_x^{-a/2,-b}}{\varepsilon_{-a/2,-b/2}} - \frac{H_x^{-a/2}}{\varepsilon_{-a/2,-b/2}} - \frac{H_x^{a/2,-b}}{\varepsilon_{a/2,-b/2}} + \frac{H_x^{a/2}}{\varepsilon_{a/2,-b/2}} \right)$$
$$+ \left(\frac{H_z^{-b,-c/2}}{\varepsilon_{-b/2,-c/2}} - \frac{H_z^{-c/2}}{\varepsilon_{-b/2,-c/2}} - \frac{H_z^{-b,c/2}}{\varepsilon_{-b/2,c/2}} + \frac{H_z^{c/2}}{\varepsilon_{-b/2,c/2}} \right),$$

$G_z^{-c/2}$

$$\approx \left(\frac{H_z^{-c/2}}{\varepsilon_{-a/2,-c/2}} + \frac{H_z^{-c/2}}{\varepsilon_{a/2,-c/2}} + \frac{H_z^{-c/2}}{\varepsilon_{-b/2,-c/2}} + \frac{H_z^{-c/2}}{\varepsilon_{b/2,-c/2}} \right)$$
$$- \left(\frac{H_z^{-a,-c/2}}{\varepsilon_{-a/2,-c/2}} + \frac{H_z^{a,-c/2}}{\varepsilon_{a/2,-c/2}} + \frac{H_z^{-b,-c/2}}{\varepsilon_{-b/2,-c/2}} + \frac{H_z^{b,-c/2}}{\varepsilon_{b/2,-c/2}} \right)$$
$$+ \left(\frac{H_x^{-a/2,-c}}{\varepsilon_{-a/2,-c/2}} - \frac{H_x^{-a/2}}{\varepsilon_{-a/2,-c/2}} - \frac{H_x^{a/2,-c}}{\varepsilon_{a/2,-c/2}} + \frac{H_x^{a/2}}{\varepsilon_{a/2,-c/2}} \right)$$
$$+ \left(\frac{H_y^{-b/2,-c}}{\varepsilon_{-b/2,-c/2}} - \frac{H_y^{-b/2}}{\varepsilon_{-b/2,-c/2}} - \frac{H_y^{b/2,-c}}{\varepsilon_{b/2,-c/2}} + \frac{H_y^{b/2}}{\varepsilon_{b/2,-c/2}} \right).$$

Summing these terms together shows that all the 96 elements exactly cancel out to zero. The discrete transversality condition of the present formulation is thus proved.

Appendix B: Discretized Equations for the Eigenvalue Problem

The complete finite difference formulation of the discretization matrix **A** in eq. (12) is presented as follows:

$(L_{xx}H_x)_{a/2}$

$$\approx \frac{1}{h^2} \left(\frac{H_x^{a/2}}{\varepsilon_{a/2,-b/2}} + \frac{H_x^{a/2}}{\varepsilon_{a/2,b/2}} + \frac{H_x^{a/2}}{\varepsilon_{a/2,-c/2}} + \frac{H_x^{a/2}}{\varepsilon_{a/2,c/2}} \right)$$
$$- \frac{1}{h^2} \left(\frac{H_x^{a/2,-b}}{\varepsilon_{a/2,-b/2}} + \frac{H_x^{a/2,b}}{\varepsilon_{a/2,b/2}} + \frac{H_x^{a/2,-c}}{\varepsilon_{a/2,-c/2}} + \frac{H_x^{a/2,c}}{\varepsilon_{a/2,c/2}} \right),$$

$(L_{xy}H_y)_{a/2}$

$$\approx \frac{1}{h^2} \left(\frac{H_y^{-b/2}}{\varepsilon_{a/2,-b/2}} - \frac{H_y^{a,-b/2}}{\varepsilon_{a/2,-b/2}} - \frac{H_y^{b/2}}{\varepsilon_{a/2,b/2}} + \frac{H_y^{a,b/2}}{\varepsilon_{a/2,b/2}} \right),$$

$(L_{xz}H_z)_{a/2}$

$$\approx \frac{1}{h^2} \left(\frac{H_z^{-c/2}}{\varepsilon_{a/2,-c/2}} - \frac{H_z^{a,-c/2}}{\varepsilon_{a/2,-c/2}} - \frac{H_z^{c/2}}{\varepsilon_{a/2,c/2}} + \frac{H_z^{a,c/2}}{\varepsilon_{a/2,c/2}} \right),$$

$(L_{yx}H_x)_{b/2}$

$$\approx \frac{1}{h^2} \left(\frac{H_x^{-a/2}}{\varepsilon_{-a/2,b/2}} - \frac{H_x^{-a/2,b}}{\varepsilon_{-a/2,b/2}} - \frac{H_x^{a/2}}{\varepsilon_{a/2,b/2}} + \frac{H_x^{a/2,b}}{\varepsilon_{a/2,b/2}} \right),$$

$(L_{yy}H_y)_{b/2}$

$$\approx \frac{1}{h^2} \left(\frac{H_y^{b/2}}{\varepsilon_{-a/2,b/2}} + \frac{H_y^{b/2}}{\varepsilon_{a/2,b/2}} + \frac{H_y^{b/2}}{\varepsilon_{b/2,-c/2}} + \frac{H_y^{b/2}}{\varepsilon_{b/2,c/2}} \right)$$
$$- \frac{1}{h^2} \left(\frac{H_y^{-a,b/2}}{\varepsilon_{-a/2,b/2}} + \frac{H_y^{a,b/2}}{\varepsilon_{a/2,b/2}} + \frac{H_y^{b/2,-c}}{\varepsilon_{b/2,-c/2}} + \frac{H_y^{b/2,c}}{\varepsilon_{b/2,c/2}} \right),$$

$(L_{yz}H_z)_{b/2}$

$$\approx \frac{1}{h^2} \left(\frac{H_z^{-c/2}}{\varepsilon_{b/2,-c/2}} - \frac{H_z^{b,-c/2}}{\varepsilon_{b/2,-c/2}} - \frac{H_z^{c/2}}{\varepsilon_{b/2,c/2}} + \frac{H_z^{b,c/2}}{\varepsilon_{b/2,c/2}} \right),$$

$(L_{zx}H_x)_{c/2}$

$$\approx \frac{1}{h^2} \left(\frac{H_x^{-a/2}}{\varepsilon_{-a/2,c/2}} - \frac{H_x^{-a/2,c}}{\varepsilon_{-a/2,c/2}} - \frac{H_x^{a/2}}{\varepsilon_{a/2,c/2}} + \frac{H_x^{a/2,c}}{\varepsilon_{a/2,c/2}} \right),$$

$(L_{zy}H_y)_{c/2}$

$$\approx \frac{1}{h^2} \left(\frac{H_y^{-b/2}}{\varepsilon_{-b/2,c/2}} - \frac{H_y^{-b/2,c}}{\varepsilon_{-b/2,c/2}} - \frac{H_y^{b/2}}{\varepsilon_{b/2,c/2}} + \frac{H_y^{b/2,c}}{\varepsilon_{b/2,c/2}} \right),$$

$(L_{zz}H_z)_{c/2}$

$$\approx \frac{1}{h^2} \left(\frac{H_z^{c/2}}{\varepsilon_{-a/2,c/2}} + \frac{H_z^{c/2}}{\varepsilon_{a/2,c/2}} + \frac{H_z^{c/2}}{\varepsilon_{-b/2,c/2}} + \frac{H_z^{c/2}}{\varepsilon_{b/2,c/2}} \right)$$
$$- \frac{1}{h^2} \left(\frac{H_z^{-a,c/2}}{\varepsilon_{-a/2,c/2}} + \frac{H_z^{a,c/2}}{\varepsilon_{a/2,c/2}} + \frac{H_z^{-b,c/2}}{\varepsilon_{-b/2,c/2}} + \frac{H_z^{b,c/2}}{\varepsilon_{b/2,c/2}} \right).$$

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