Direct visualization of photonic band structure for three-dimensional photonic crystals

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We propose a method to experimentally determine the full photonic band structure of photonic crystals by monitoring the beam propagation, and we demonstrate the experimental results of the band-structure measurement in the near-infrared regime for Si/SiO_2 three-dimensional hexagonal photonic crystals fabricated by autocloning bias-sputtering process.

Photonic crystals (PhC's) have a great potential on photonics technology because a photonic insulator— which had been believed to be nonexistent—can be realized if a PhC possesses a full photonic band gap.[1] In addition, light propagation in PhC's can be tuned to a large extent beyond the limitation of real materials by tuning their crystal structure. In other words, PhC's enable band engineering in photonics, by which we can artificially control the optical properties of solids.[2] To study or design a PhC (to design light-propagation properties or to modify the width or anisotropy of the forbidden band), it is essentially important to know its band structure, just as one must know the electronic band structure to understand the electronic properties of a solid. This is especially important for the fabrication of three-dimensional (3D) full photonic band-gap materials in the optical wavelength regime, which is still a difficult task even with state-of-the-art technology. We have to carefully examine the band structure of PhC's that can be fabricated by available techniques, and have to know how to modify the structure to widen the partial gap to a full gap. This task is impossible without the knowledge of PhC's band structure.

From the viewpoint of theorists, various methods have been developed to calculate photonic bands,[3] and it is not very difficult to calculate them with a sufficient computer if the exact crystal structure is known. From the viewpoint of experimentalists, however, it is not so easy to directly measure the photonic band structure, especially in the visible and near-infrared regime. Although there have been many reports on transmittance and/or reflectivity measurements, they are not directly related to the band structure; they are more closely related to the density of states.[4] In the microwave regime, a coherent phase-sensitive measurement can provide the band-structure information,[5] but such a method cannot be applied in the optical regime.

The direct measurement of the photonic band structure is especially important when the exact crystal structure is difficult to know[6] or the finite size effect is unnegligible (e.g., a quasi-two-dimensional PhC of finite thickness). In such cases, we have to rely on direct measurement. Furthermore, when designing the beam propagation properties of PhC's, it is not sufficient to know the band structure in some high-symmetry axes, which is usually done in band calculation. It is crucial to know the *full* band structure, i.e., that not restricted within high-symmetry axes, because the propagation direction is determined by the band curvature in the k space.[7]

The fact that beam propagation is influenced by the complicated band structure leads to various anomalous propagation phenomena recently observed in grating waveguides[8] and photonic crystals.[9] Since such propagation properties contain the information of the photonic band (this propagation mode is referred to as the Bloch mode[10]), the possibility of experimental reconstruction of the band structure by similar beam propagation experiments is suggested. However, it is not clear whether such a method really works because it is unclear whether such propagation experiment data are sufficient for reconstructing the full band structure and also because the reported experimental results were not fully quantitatively explained by the band-structure calculation. For example,[9] many of the observed modes propagate in the opposite direction from that predicted by the band-structure calculation, and the deviation from theory is not small, especially in the region far from the Bragg condition. These indicate that reconstruction is not reliable.

In this paper we show the quantitative relationship between the beam propagation and the band structure in PhC's, and propose a versatile method for measuring the *full* photonic band structure, in which we reconstruct the band structure from beam propagation experiments. This method enables us to obtain the complete relationship between ω and k for all directions. Furthermore, we demonstrate the experimental results on alternating-layer 3D PhC's fabricated by autocloning bias-sputtering process in near-infrared wavelengths.

When an optical beam is launched from a material 1 (air) to a material 2 (dielectric), the beam propagation in the material 2 is determined by the conservation law of tangential components of wave vector k. This conservation law can be graphically represented by plotting the equifrequency surface (EFS) and a normal line in the k space, as shown in Figs. 1(a) and 1(b). In the case for the dielectric, EFS is a sphere, and the k conservation leads to Snell's law. If material 2 is a PhC [Fig. 1(c)], Snell's law does not hold, but the beam propagation direction is still governed by the k conservation with some modifications to the dielectric case. First, in PhC's, EFS should be infinitely periodic in the k space.[11] In Ref. 9 they considered EFS only within the first Brillouin zone

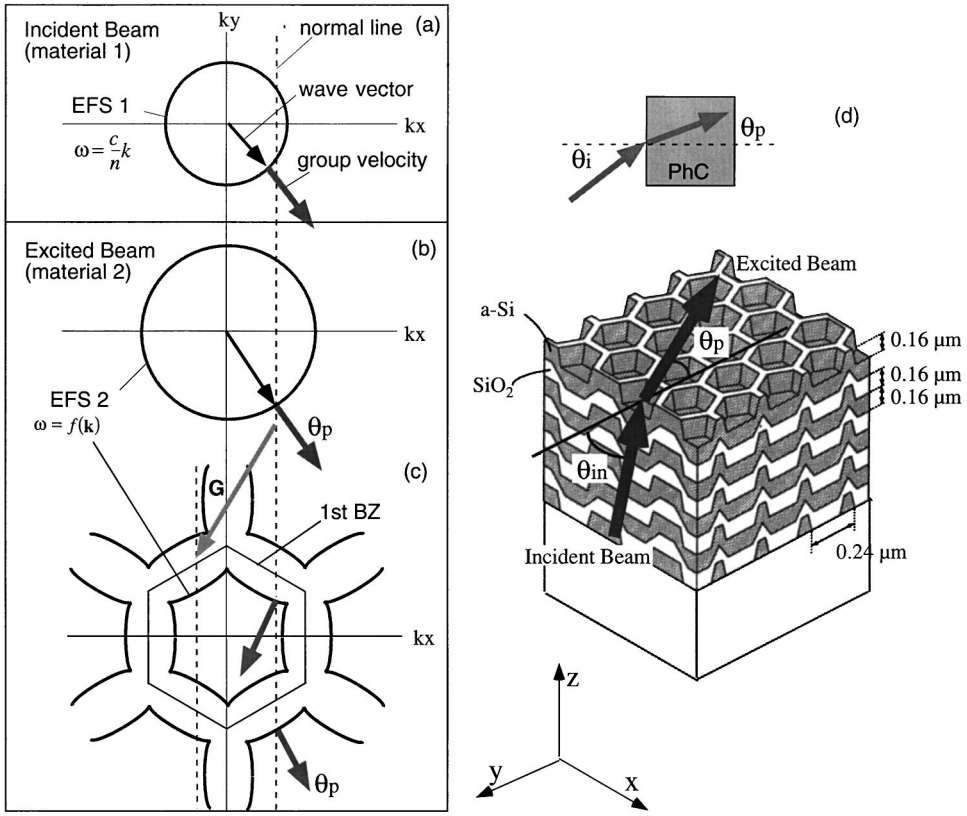

FIG. 1. (a)–(c) Schematics of the EFS plot for the beam incident problem. (d) The measurement setup and the 3D PhC sample fabricated by autocloning bias sputtering.

(BZ), but it is not generally clear whether the first BZ is sufficient. Furthermore, the propagation direction in the PhC's is determined by the group velocity of Bloch modes, which is related to the band structure and EFS by $v_g = \mathrm{grad}_k(\omega)$.[7] (Here we assume that the propagation direction is always the same as the group velocity, not in the opposite direction.)

For the beam propagation experiment, we measure the incident and propagating angles (θ_{in} and θ_p). θ_{in} determines the tangential component of k provided the refractive index of the outside media (normally air) is known, and θ_p determines the orientation of group velocity, which corresponds to the normal direction of the EFS, and is expressed as $dk_y/dk_x = \tan(\theta_p)$. Thus, we can estimate the EFS by integrating the propagation angle in the k space. One may notice that there is uncertainty in determining the EFS due to the arbitrariness of the integration constant. However, if the symmetry of the PhC is known, the EFS can be unambiguously determined. Note that the knowledge of the crystal symmetry is also required when we apply the generalized conservation rule mentioned above. If the symmetry is unknown, it can be determined by an optical beam diffraction,[12] which is analogous to x-ray diffraction measurement for determining the crystal structure of a solid.

Consequently, the actual band determination procedure is the following: first integrate the angle data to obtain a part of the EFS, and then regenerate other parts of the EFS from the first one with considering the crystal symmetry. We repeat this until further regeneration does not change the shape of the EFS within the first BZ. In this procedure, the extended zone scheme is essential to construct the EFS. We will discuss this point again after we analyze the experimental data. By this procedure, the unknown EFS can be determined by the beam propagation measurement. This method may be regarded as a photonic counterpart to cyclotron resonance measurements on metals, which provide information on the Fermi surface. In contrast to Fermi energy, we can vary ω almost arbitrarily with the help of a tunable laser. This enables us to determine the shape of the EFS as a function of ω, which means that we can know the *full* band structure, that is, the complete relationship between ω and k in all directions.

Figure 1(d) shows how the measurement is carried out. A nearly collimated beam is launched from a wavelength-tunable Ti:sapphire laser to a PhC. θ_p is measured by a charge-coupled device (CCD) camera monitoring from the z direction as a function of θ_{in}. The sample was a Si/SiO_2 alternating-layer 3D hexagonal PhC fabricated by *autocloning* bias-sputtering deposition.[13] We wrote a 2D hexagonal pattern by e-beam lithography and transferred it to a SiO_2 layer on an InP substrate by dry etching. a-Si/SiO_2 layers were then deposited alternatively on this patterned substrate. By choosing the appropriate sputtering condition, the surface of layers takes on a certain stable shape after a few layer deposition, and each layer deposited hereafter keeps the 2D periodic pattern even until 40-layer deposition. This autocloning deposition results in a 3D hexagonal PhC structure. We used a 40-layer PhC with an in-plane lattice constant a of 0.24 μm. The thickness of each layer was 0.16 μm. The unit structure is composed of complicated tilted and bent surfaces. The beam incident interface is the x-z plane, perpendicular to the Γ-K direction, and the incident plane is the x-y plane. Furthermore, the incident beam has p polarization in which electric field lies within the incident plane.

Figure 2 shows the relation between θ_{in} and θ_p at 0.86 μm. The measured relationship is far different from the

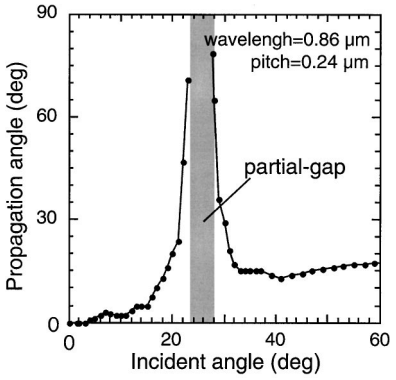

FIG. 2. Incident angle versus the propagating angle at $\lambda = 0.86\ \mu$m.

Snell's law and should be attributed to the complicated EFS shape. Between 21.5°–28° (shaded area), the beam propagation was not observed, which indicates the existence of a partial gap in the photonic band. By integrating these angle data, we constructed the EFS at each frequency assuming hexagonal symmetry. Figure 3(a) shows a deduced EFS in the k space at 0.86 μm. The raw data correspond to the shaded region, and other branches are the result of regeneration. Note that the raw data are located outside the first BZ. This shows that the extended zone scheme (inclusion of the zone outside the first BZ) is essential to quantitatively understand the relationship between the beam propagation and the band structure. The starlike shape in the first BZ reflects the in-plane symmetry of the PhC at symmetry points in the k space. Figure 3(b) shows an EFS at 0.93 μm. In 3(b), there are partial gaps (as indicated by an arrow) around K points. The beam propagation is most strongly altered around these partial gaps; the group velocity of the Bloch photons becomes slow and the propagation angle significantly differs from Snell's law due to strong multiple scattering. For realizing a full photonic band gap, we have to enlarge these partial gaps centered at symmetry points. When integrating the experimental data, the EFS becomes discontinuous and uncertain at symmetry points due to the appearance of gaps. But if we take the known symmetry of the PhC into account, we can safely determine the integration constant with the help of the knowledge of the symmetry around such symmetry points.

Since Fig. 3 is a cross section of the full band structure at each ω, we can construct the band structure by sweeping ω. Figure 4 plots the full band structure around the K point between 0.84–0.96 μm. We introduce here normalized frequency $\omega = 2\pi c/a$. For a clear view of the bands near the K point, the other branches far from the K point are not plotted. A clear gap appears around 0.92 μm between the upper and lower bands. Both bands exhibit threefold rotational symmetry of the K point. Note that the symmetry axis differs by 180° between the upper and lower bands. By this method, we can measure the relation between ω-(k_x, k_y). In the present case, the small area of (k_x, k_y) around the M point is out of the measurable range because the refractive index difference between air and the Si/SiO_2 PhC is too large. But if we perform a supplementary measurement in which the incident interface lies in the y-z plane (that is, rotating the sample by 90°), any point of (k_x, k_y) becomes accessible. In addition, if

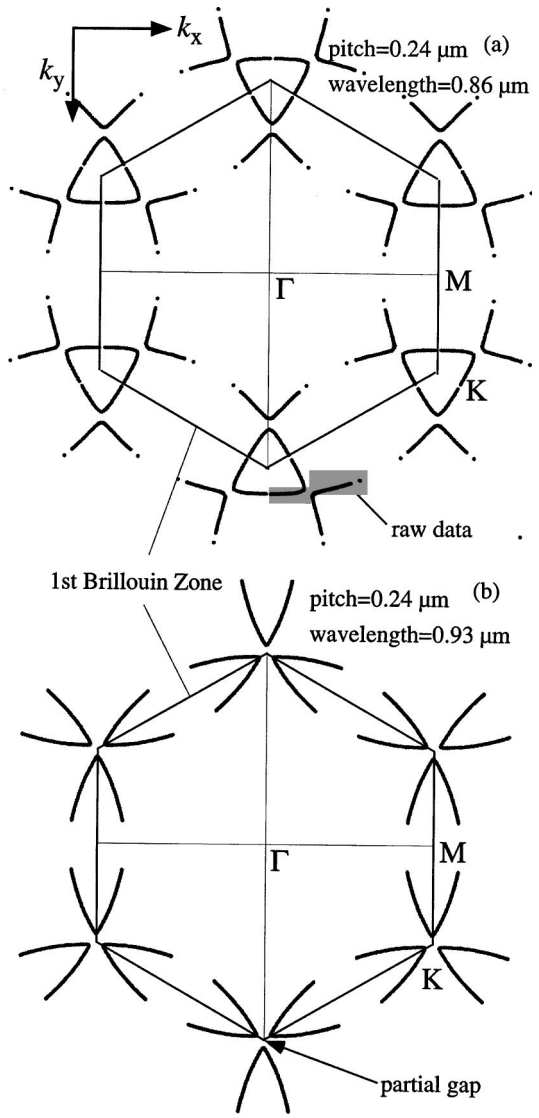

FIG. 3. Experimentally determined EFS's of the 3D PhC in the k_x-k_y plane at (a) $\lambda = 0.92$ and (b) $\lambda = 0.86$.

we change the incident plane to the x-z or y-z plane, we can measure (k_x, k_y, k_z) points with nonzero k_z.

Next, we compare the experimental data with calculations. We calculated the band structure of the present 3D PhC in typical high-symmetry axes assuming an approximated hexagonal shape by a full vector calculation with the plane-wave expansion method.[14] Figure 5 shows (a) experimentally determined and (b) calculated band structure for high-symmetry directions (Γ-K-M) in the case of p polarization.[15] The measured results are basically similar to the calculated ones, which shows the feasibility of our measurement method. Since it is difficult to know the accurate 3D shape and index profile of the present PhC, we believe that the measured band structure is *closer* to the real band structure than the calculated one. In addition, this agreement denies the existence of any anomalous modes propagating in the opposite direction to the group velocity in our result.

In the above discussion we discussed only the k conservation, but the amplitude of the field should be conserved as well, which is not included in the framework of the EFS plot. The amplitude conservation determines the amplitude ratio

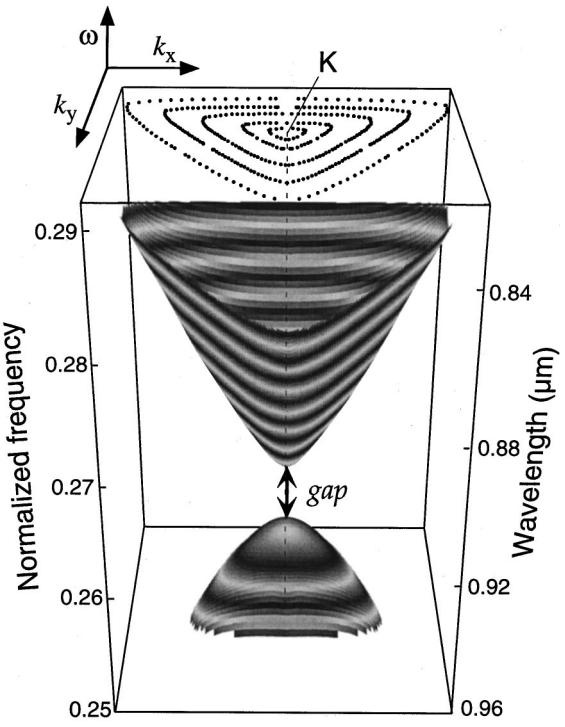

FIG. 4. Experimentally determined photonic band structure around the K point in the ω-(k_x-k_y) space.

of the allowed Bloch modes. This means that some of Bloch modes allowed in the EFS plot are not practically excited. In our experiment the number of the observed modes is smaller than that of the allowed Bloch modes in the EFS plot, probably because the amplitude of some modes is too small to be observed or practically zero. But it is not necessary to measure all of the Bloch modes, and the number of the observable modes is sufficient for PhC's with high symmetry to construct the full band structure because many of the allowed modes are equivalent due to their symmetry.

We end this article with comments on the accuracy and versatility of this method. This accuracy mainly relies on the accuracy of θ_p. This uncertainty leads to the uncertainty of k_y as $\Delta k_y \approx k_x \tan\theta_p \Delta\theta_p$ (Δk_x is negligible). θ_p is limited by the beam width and the sample size, which are approximately 30 and 500 μm in our case. Although the error can be

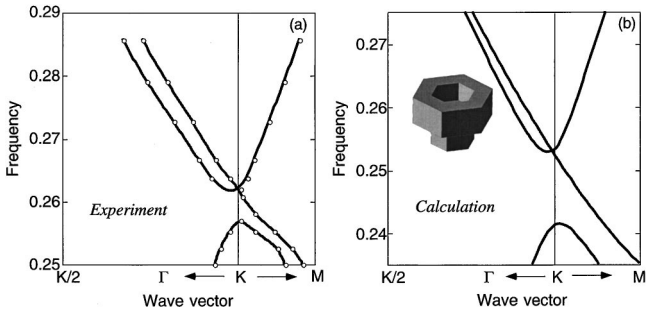

FIG. 5. (a) Experimentally determined photonic band for high-symmetry directions. (b) Calculated band structure for high-symmetry directions. About 1200 plane waves per each polarization were used in the calculation. The inset shows the approximated shape of the 3D PhC used in this calculation. Frequency is normalized as $\omega = 2\pi c/a$.

large when θ_p is large, we can safely avoid such data by using the crystal symmetry. The error of k_y/k_x is less than 4% in our case. Of course, this can be further improved if we use a smaller beam and larger samples.

This method relies on the existence of weak scattering light for the vertical direction, which may limit the versatility of this method. We think that most of bulk 2D/3D PhC's with sufficiently small thickness meet this demand if we use a sufficiently intense laser beam. If the PhC is embedded within some waveguiding structures, such scattering light may not be detected. But the propagation angle can still be determined by monitoring the beam position at the output edge of the PhC's.

In summary, we have shown that the exact shape of the EFS can be deduced from a beam propagation measurement. This method with a tunable light source enables the experimental determination of the full photonic band structure. Not only can the band along high-symmetry axes be determined, but we can also determine any points in bands within the incident plane, which is important to understand various aspects of propagation phenomena in PhC's. We have demonstrated successful measurements of an alternating-layer 3D hexagonal PhC fabricated by autocloning bias sputtering.

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[1] E. Yablonovitch, Phys. Rev. Lett. **58**, 2059 (1987).
[2] J. D. Joannopoulos, R. D. Meade, and J. N. Winn, *Photonic Crystals* (Princeton University Press, New Jersey, 1996).
[3] J. W. Haus, J. Mod. Opt. **41**, 195 (1994).
[4] For example, S. Y. Lin *et al.*, Nature (London) **394**, 251 (1998).
[5] W. M. Robertson *et al.*, Phys. Rev. Lett. **68**, 2023 (1992).
[6] S. G. Romanov *et al.*, Appl. Phys. Lett. **70**, 2091 (1997).
[7] K. Ohtaka *et al.*, J. Phys. Soc. Jpn. **65**, 3068 (1996).
[8] P. St. J. Russell and T. A. Birks, in *Photonic Band Gap Materials*, edited by C. M. Soukoulis (Kluwer Academic, Dordrecht, 1996).
[9] H. Kosaka *et al.*, Phys. Rev. B **58**, R10 096 (1998).
[10] A. Yariv and P. Yeh, *Optical Waves in Crystals* (Wiley, New York, 1984).
[11] This extended zone scheme is equivalent to a generalized k-conservation rule in which the tangential component of $k + G$ (G is a reciprocal vector) is conserved [shown by a short vertical broken line in Fig. 1(c)]. We regard that the extended zone scheme is more useful in reconstructing the EFS than the generalized k-conservation rule.
[12] For example, I. I. Tarhan and G. H. Watson, Phys. Rev. Lett. **76**, 315 (1996).
[13] S. Kawakami, Electron. Lett. **33**, 1260 (1997).
[14] K. M. Ho *et al.*, Phys. Rev. Lett. **65**, 3152 (1990).
[15] We classified the calculated eigenmodes by their dominant polarization components. Due to its layer-by-layer-like structure, most of the Bloch modes in the present PhC can be classified as s or p polarization.