Defect modes in a two-dimensional square lattice of square rods

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We investigated defect modes created by drilling a hole in a rod and rotating it in a two-dimensional square lattice of square dielectric rods as well as that of square metallic rods in air by the supercell method. In E polarization (the electric field parallel to the rod axis), a hole in a dielectric rod created a nondegenerate acceptor mode inside the photonic band gap (PBG), while the one in a metallic rod resulted in a nondegenerate donor mode below the cutoff frequency. The frequency of the acceptor mode extends almost all over the PBG. The rotation of a square rod did not create defect modes in either case, regardless of the angle of rotation. In H polarization (the magnetic field parallel to the rod axis), a hole in the dielectric rod created acceptor modes and rotating the rod resulted in paired donor and acceptor modes. As the angle of rotation increased, the donor mode moved away from the top of the PBG and the acceptor mode moved away from the bottom of the PBG. One of the defect modes of H polarization was strongly localized around the rods surrounding the defect rod rather than around the defect rod itself. [S1063-651X(98)13811-4]

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I. INTRODUCTION

Photonic crystals, which are periodic arrays of dielectric materials, can exhibit frequency regions where electromagnetic waves cannot propagate in any direction. These frequency regions are called photonic band gaps (PBG's), analogous to electronic band gaps in semiconductors [1,2]. Photonic crystals can be used in high-efficiency semiconductor lasers and in light-emitting diodes, optical diodes, solar cells, optical switches, and high-Q resonant cavities.

Photonic crystals have very useful and attractive properties that semiconducting crystals do not. Defects in photonic crystals are easily created by either adding or removing dielectric material from a chosen unit cell in the crystals. Thus the defect frequency inside a PBG can, in principle, be selected by designing the shape or the size of a local defect in photonic crystals. Previous studies have reported that local defects created by reducing the dielectric constant of one of the artificial dielectric atoms in photonic crystals or by removing the dielectric material from the crystals produce acceptor modes at the bottom of a PBG. On the other hand, those created by increasing the dielectric constant or by locally adding an extra dielectric material produce donor modes at the top of a PBG [3,4]. In photonic crystals of metallic materials (metals, heavily doped semiconductors, or superconductors), it has been observed that local defects create defect modes below the cutoff frequency ω_c [5–7]. Recently, it was shown that the defect frequency approaches ω_c as the radius of local defects created by removing metallic material in a layer-by-layer metallic PBG structure is increased; this is also the case of acceptor modes produced by removing the dielectric material in dielectric photonic crystals [8]. Defect modes may play an important role in the application of photonic crystals to semiconductor lasers and high-Q cavities [3,8]. To date, experimental investigations on defects in two-dimensional (2D) photonic crystals have primarily been performed with structures obtained by removing dielectric or metallic cylinders [6,9]. These defects are similar to the vacancies in semiconductors. Defects can be also created in 2D photonic crystals by changing the shape or the size of one of the artificial dielectric atoms or by replacing it with different dielectric materials. The former method is more suitable to 2D photonic crystals since the etching technology can be best employed to realize the desired structure.

In this paper we propose a simple method of creating defect modes and investigate the modes created thereby. Our method was to drill a hole at the center of a rod placed at the center of a 2D square lattice consisting of either square dielectric rods or square metallic rods in air. It has been recently reported that a 2D square lattice of square dielectric rods in air opens an absolute PBG in higher-frequency regions [10]. The role of the hole in a dielectric rod will be different from that in a metallic rod because the dielectric constant of the dielectric rod is larger than that of the hole, while that of the metallic rod is smaller. We also investigated defect modes created by rotating a square rod placed at the center of 2D square photonic crystals. Because the rotation of the rod in effect moves dielectric material from one side to the other, the properties of this local defect are expected to be different from those of defects investigated until now. In Sec. II we describe our calculational model and method. We present and discuss the defect modes created by the hole and rod rotation in Secs. III A and III B, respectively. In Sec. IV we summarize the conclusions of this study.

II. CALCULATIONAL MODEL AND METHOD

For the purposes of this study we considered 5×5 supercells, each containing 25 square dielectric rods (a dielectric supercell) and square metallic rods (a metallic supercell). A defect rod was placed at the center of the supercells. Increasing the supercell size may make defect bands slightly narrower, but will not change its position inside the PBG.

The supercell method was employed to calculate defect modes inside the PBG [3]. We considered E polarization (the electric field parallel to the rod axis) only for square metallic rods because PBG's do not exist in H polarization (the mag-

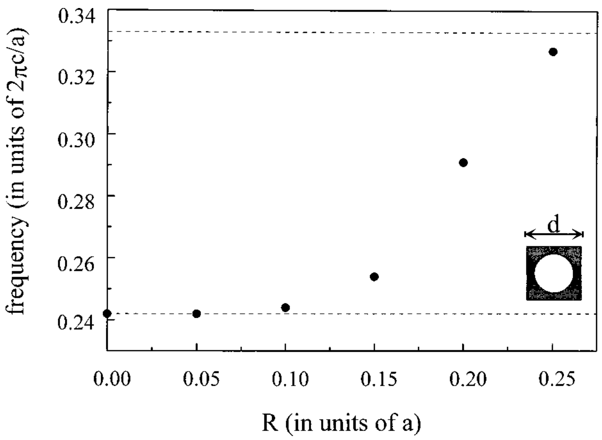

FIG. 1. Frequency dependence of the defect mode of E polarization in a dielectric supercell on the hole radius R normalized to the lattice constant a of the conventional square lattice. This is a nondegenerate acceptor mode. The frequency is normalized to $2\pi c/a$ and the width d of the square rod is $0.5a$. The inset denotes the defect rod.

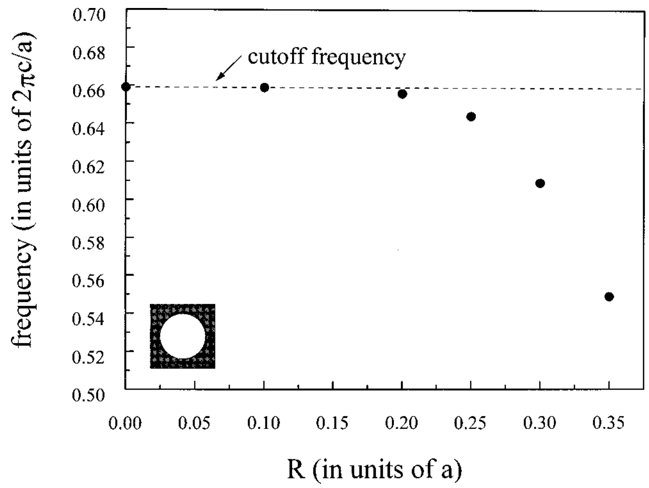

FIG. 2. Frequency dependence of the defect mode of E polarization in a metallic supercell on the hole radius R normalized to a. It is a nondegenerate donor mode. The width of the square rod is $0.75a$.

netic field parallel to the rod axis) in 2D metallic composites [11]. The dielectric constant of metallic rods was assumed to be the free-electron form $\epsilon(\omega)=1-\omega_p^2/\omega^2$, where ω_p is the plasma frequency of the square metallic rod. The number of plane waves used in the E polarization was 6361, which corresponds to 253 plane waves for the conventional square lattice. Since we consider the PBG below the second band, this number yields values that converge well. For H polarization the number of plane waves used in the calculations was 7087, corresponding to 305 plane waves for the conventional square lattice, since the first PBG exists between the sixth and the seventh bands [10]. In both polarizations the PBG's calculated for supercells without the defect rod agreed well with those calculated by using the plane waves for the conventional square lattice.

III. RESULTS AND DISCUSSION

A. Defect modes created by a hole

Figure 1 shows the frequency dependence of a defect mode of E polarization in a dielectric supercell on the hole radius R normalized to the lattice constant a of the conventional square lattice. Two dashed lines in the figure denote the first PBG between the M point of the first band and the X point of the second band for the conventional square lattice when the width d of the square dielectric rod is $0.5a$ and the dielectric constant of the rod is 12.25. The frequency is normalized to $2\pi c/a$, where c is the vacuum velocity of light. The inset denotes the defect rod. As expected, making a hole in the rod creates an acceptor mode, which is always nondegenerate. As the hole radius is increased, the frequency of the defect mode approaches the upper edge of the PBG, i.e., it becomes the deeper acceptor mode. There exists a threshold radius of the hole required to create an acceptor mode; this is about $0.1a$. When the hole radius is $0.2a$, the frequency of the acceptor mode is placed near the center of the PBG. For example, when $a=1.0$ μm, $d=0.5$ μm, and $R=0.2$ μm, the PBG lies in the region $\lambda=4.13-3.01$ μm and the corresponding defect wavelength is $\lambda=3.44$ μm. We notice that the frequency of the acceptor mode extends almost throughout the PBG. Since etching technology on a submicrometer scale simplifies making a hole at the center of a square rod, this method is potentially useful in the application of 2D photonic crystals to semiconductor lasers.

Figure 2 shows the frequency dependence of the defect mode of E polarization in a metallic supercell on the hole radius R normalized to a; the frequency is also normalized to $2\pi c/a$. The dashed line denotes the cutoff frequency ω_c and the inset the defect rod. The width of the square metallic rod is $0.75a$ and ω_p is assumed to be unity in units of $2\pi c/a$. In contrast to the dielectric supercell, a hole introduces a nondegenerate donor mode below ω_c. As the hole radius increases, the frequency of the defect mode moves farther away from the cutoff frequency, becoming the deeper donor mode. There is also the threshold radius of almost $0.2a$ for a hole required to create the donor mode. This behavior is different from that of the three-dimensional layer-by-layer metallic PBG structure [8]. The defect mode of E polarization created by the hole is nondegenerate in both supercells because it originated in the first nondegenerate band. The role of the hole in dielectric and metallic rods is analogous to that of group IV dopants in III-V semiconductors.

Figure 3(a) shows the spatial distribution of the squared electric field (the electric energy density) of the acceptor mode in the dielectric supercell when the hole radius is $0.2a$ and Fig. 3(b) that of the donor mode in the metallic supercell when the hole radius is $0.35a$. The electromagnetic field is strongly localized around the defect rod, as expected for a localized defect mode in the dielectric supercell. It has been pointed out that the oscillation of the localized field [i.e., the satellite peaks in Fig. 3(a)] shows the interference or the standing-wave pattern of the electric energy density generated by defect scattering [9]. The decay length of the localized acceptor mode was determined to be $0.644a$ from the central peak. Interestingly, in the metallic supercell the electromagnetic field is also localized around the defect rod with no oscillation present; this can be explained by the fact that

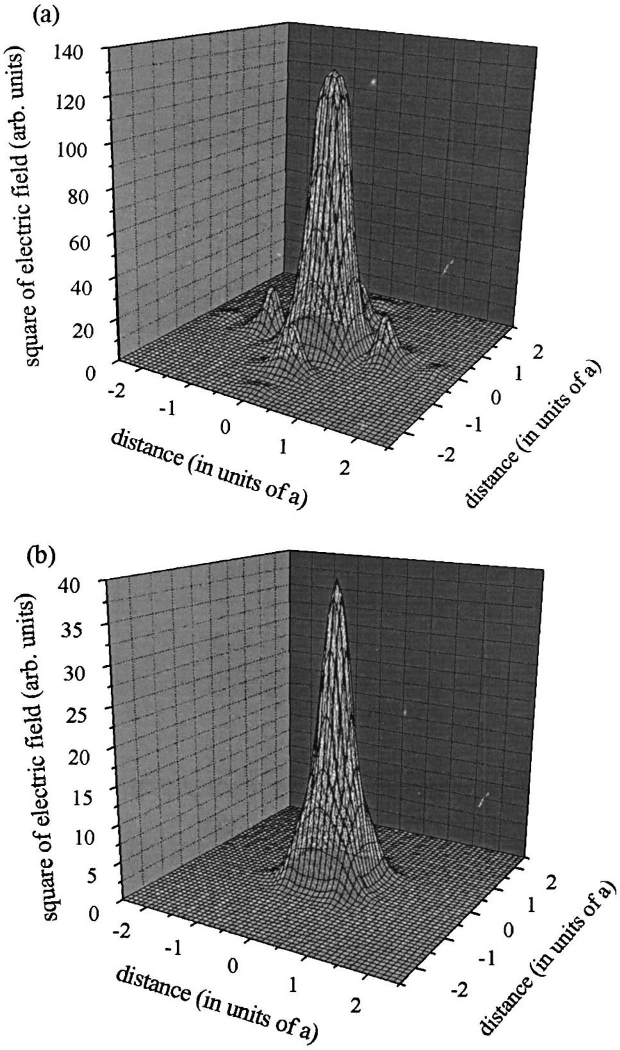

FIG. 3. Spatial distribution of the squared electric field of (a) the acceptor mode of E polarization in the dielectric supercell when the width of the square rod is $0.5a$ and the hole radius is $0.2a$ and (b) the donor mode of E polarization in a metallic supercell when the width of the square rod is $0.75a$ and the hole radius $0.35a$.

metallic materials prevent electromagnetic fields from interacting with each other.

Defect modes of H polarization created by a hole are complex and interesting. Figure 4 shows the frequency dependence of the defect mode of H polarization in a dielectric supercell on the hole radius R normalized to a. The two dashed lines in Fig. 4 denote the first PBG between the Γ point of the sixth band and the M point of the seventh band for the conventional square lattice when the width d of the square dielectric rod is $0.64a$ and its dielectric constant is 12.25. Since the PBG is the gap between the higher bands, a large number of defect modes appear in the PBG when the hole radius is further increased, in contrast to the E polarization whose first PBG is the gap between the first and second bands [12]. The solid lines and symbols gD_i distinguish between the defect modes, where g is the degree of degeneracy of the defect mode and i is the order in which the defect mode appears inside the PBG as R increases. g is omitted when a defect mode is nondegenerate and the inset denotes the defect rod. Open circles denote doubly degenerate acceptor modes. The frequency of doubly degenerate modes $2D_2$ increases rapidly in comparison to D_1 as R increases and that of D_3 increases very slowly in comparison to D_4. These behaviors give rise to intersections of the defect modes: D_1 and $2D_2$ near $R=0.1a$ and D_3 and D_4 near $R=0.275a$.

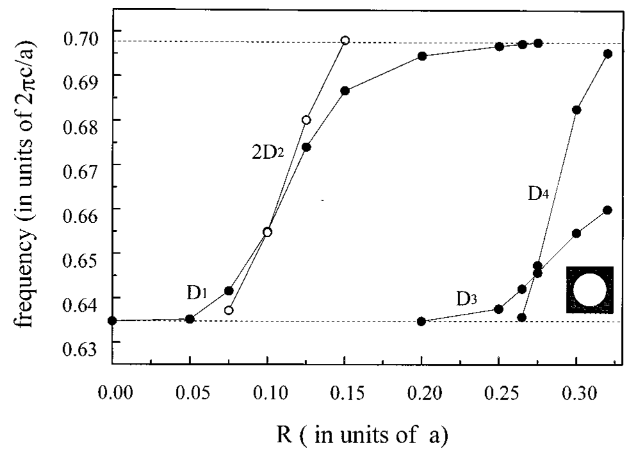

FIG. 4. Frequency dependence of the defect modes of H polarization in a dielectric supercell on the hole radius R normalized to a. The width of the square rod is $0.64a$.

Figure 5(a) shows the spatial distribution of the squared magnetic field, i.e., the magnetic energy density, of the acceptor mode D_1 of H polarization when the hole radius is $0.125a$ and Fig. 5(b) shows that of D_3 when the hole radius is $0.3a$. As expected, the electromagnetic field of D_1 is also localized around the defect rod. There is also an oscillation of the localized field, as in Fig. 3(a), for the electric energy density. Interestingly, the electromagnetic field of D_3 is not localized around the defect rod itself, but is strongly localized around the rods surrounding the defect rod. Therefore, the effect of the hole in D_3 is much smaller than those in the other defect modes. This explains well why the frequency of D_3 increases very slowly as R increases.

B. Defect modes created by rotation

Figure 6 shows the frequency of defect modes of H polarization created by rotating a square rod as a function of the rotation angle θ of the rod in a dielectric supercell. The width of the square dielectric rod is $0.64a$ and its dielectric constant 12.25. Dashed lines denote the first PBG and the inset represents the defect rod rotated by 45°. Since the rotation of a square rod moves dielectric material from one side to the other, the local defect of rotating a square rod creates a donor mode (solid circle) and an acceptor mode (open circle) in pairs, i.e., the donor-acceptor pair mode. The donor and the acceptor modes move away from the top and the bottom of the PBG as the rotation angle increases, respectively, thus becoming the deeper donor-acceptor pair mode. The frequencies of donor-acceptor pair modes at a rotation angle θ are equal to those at a rotation angle $90°-\theta$, as expected. The frequency difference between the donor and the top of the PBG is nearly equal to that between the acceptor and the bottom of the PBG. The amount of dielectric material shifted as the rod rotates by the angle θ, $\Delta S(\theta)$, is $0.25d^2\ (\epsilon_r - \epsilon_a)(\cos^{-1}\theta-1)(\sin^{-1}\theta-1)$, where ϵ_r is the dielectric constant of a square rod and ϵ_a that of air. $\Delta S(\theta)$ is maxi-

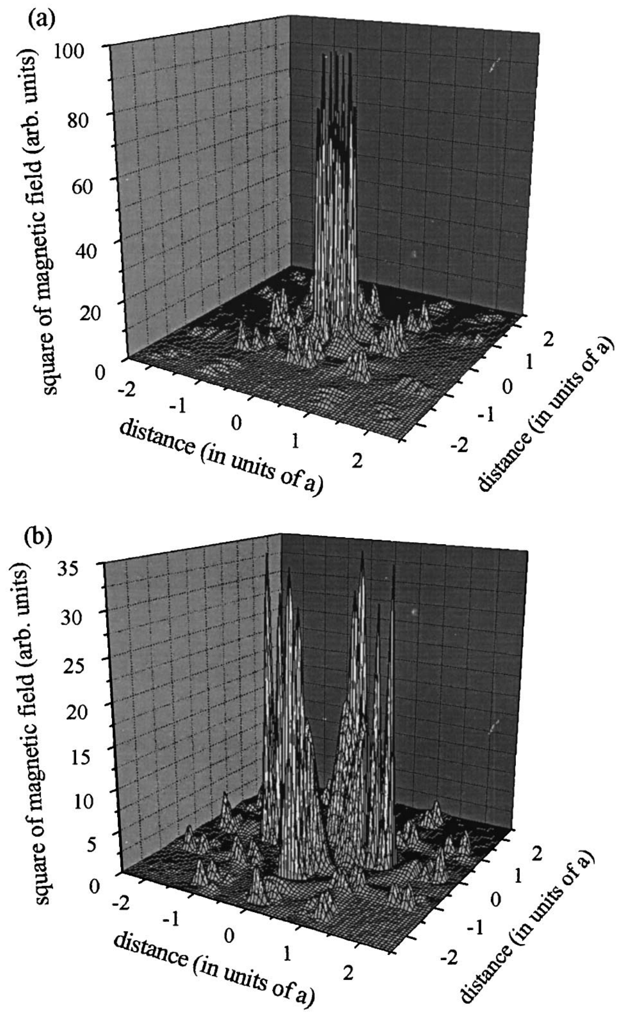

FIG. 5. Spatial distribution of the squared magnetic field of the acceptor mode (a) D_1 of H polarization in a dielectric supercell when the hole radius is $0.125a$ and (b) D_3 when the hole radius is $0.3a$. In both cases, the width of the square dielectric rod is $0.64a$.

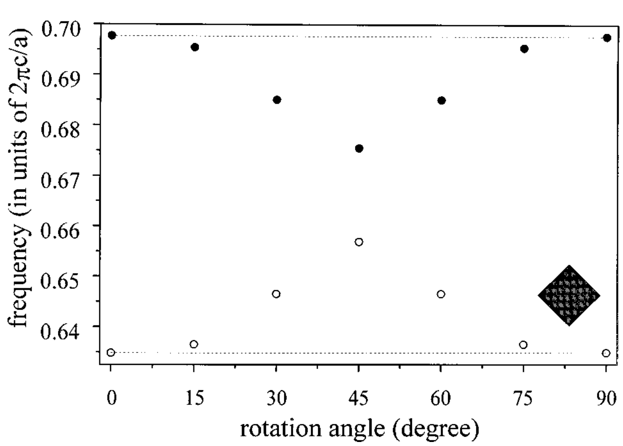

FIG. 6. Frequency of defect modes of H polarization created by rotating a square rod as a function of the rotation angle θ of the rod in a dielectric supercell. The width of the rod is $0.64a$. Solid circles denote donor modes and open circles acceptor modes. The inset denotes the rotated defect rod by $\theta=45°$.

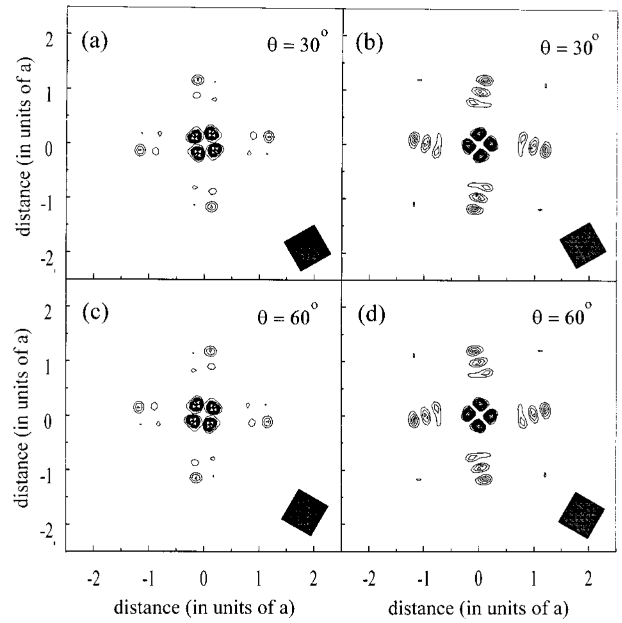

FIG. 7. Contour of the squared magnetic field of the donor-acceptor pair modes; at $\theta=30°$ (a) is for the acceptor mode and (b) the donor mode and at $\theta=60°$ (c) is for the acceptor mode and (d) the donor mode. Insets show the rotated defect rods at respective angles.

mum at $\theta=45°$ and $\Delta S(\theta)=\Delta S(90°-\theta)$, explaining well the dependence of the donor-acceptor pair mode on the rotation angle θ.

Figure 7 illustrates the contours of the squared magnetic field of the donor-acceptor pair modes. Figures 7(a) and 7(b) are those of the acceptor mode and the donor mode at $\theta=30°$, Fig. 7(c) that of the acceptor mode, and Fig. 7(d) that of the donor mode at $\theta=60°$ or $-30°$, respectively. The gray square denotes the rotated rod. The magnetic field is localized around the rotating rod and rotates in the same direction as the defect rod.

In E polarization, the rotation of a square rod cannot create defect modes in both supercells, regardless of the angle of rotation. In fact, defect modes do not exist in the PBG of E polarization. The effect of the rod shape on the PBG's in a 2D triangular photonic crystal has been previously reported [13]. In a triangular photonic crystal consisting of dielectric rods in air, it was shown that a change in the shape of rods can affect the eigenmodes of H polarization rather than those of E polarization. Thus changes in the spatial distribution of rods due to rotation dominantly affect the eigenmodes of H polarization.

IV. CONCLUSION

In conclusion, we investigated defect modes created by drilling a hole in a rod and rotating it in a 2D square lattice of square dielectric rods in air by the supercell method as well as those created in a lattice of square metallic rods. In E polarization, a hole in a dielectric rod created a nondegenerate acceptor mode inside the PBG, while in a metallic rod the hole resulted in a nondegenerate donor mode below the cut-off frequency. The frequency of the acceptor mode extended almost throughout the PBG. The rotation of a square rod did not create defect modes in either supercell, regardless of the angle of rotation. In H polarization, a hole in a dielectric rod created acceptor modes. The local defect of rotating a square rod resulted in a donor mode and an acceptor mode in pairs. The donor and the acceptor mode moved away from the top and the bottom of the PBG, respectively, as the rotation angle increased. The defect modes of E polarization were strongly localized around the defect rod, as expected. However, one of the defect modes of H polarization was strongly localized around the other rods surrounding the defect rod rather than around the defect rod itself.

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[1] K. M. Ho, C. T. Chan, and C. M. Soukoulis, Phys. Rev. Lett. **65**, 3152 (1990).
[2] E. Yablonovitch, T. J. Gmitter, and K. M. Leung, Phys. Rev. Lett. **67**, 2295 (1991).
[3] E. Yablonovitch, T. J. Gmitter, R. D. Meade, A. M. Rappe, K. D. Brommer, and J. D. Joannopoulos, Phys. Rev. Lett. **67**, 3380 (1991).
[4] R. D. Meade, A. M. Rappe, K. D. Brommer, J. D. Joannopoulos, and O. L. Alerhand, Phys. Rev. B **48**, 8434 (1993).
[5] M. M. Sigalas, C. T. Chan, K. M. Ho, and C. M. Soukoulis, Phys. Rev. B **52**, 11 744 (1995).
[6] D. R. Smith, S. Schultz, N. Kroll, M. Sigalas, K. M. Ho, and M. Soukoulis, Appl. Phys. Lett. **65**, 645 (1994).
[7] D. F. Sievenpiper, M. E. Sickmiller, and E. Yablonovitch, Phys. Rev. Lett. **76**, 2480 (1996).
[8] J. S. McCalmont, M. M. Sigalas, G. Tuttle, K. M. Ho, and C. M. Soukolis, Appl. Phys. Lett. **68**, 2759 (1996).
[9] S. L. McCall, P. M. Platzman, R. Dalichaouch, David Smith, and S. Schultz, Phys. Rev. Lett. **67**, 2017 (1991).
[10] Chul-Sik Kee, Jae-Eun Kim, and Hae Yong Park, Phys. Rev. E **56**, R6291 (1997).
[11] V. Kuzmiak, A. A. Maradudin, and F. Pincemin, Phys. Rev. B **50**, 16 835 (1994).
[12] Pierre R. Villeneuve, Shanhai Fan, and J. D. Joannopoulos, Phys. Rev. B **54**, 7837 (1996).
[13] R. Padjen, J. M. Gerard, and J. Y. Marzin, J. Mod. Opt. **41**, 295 (1994).