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Theoretical investigation of defects in photonic crystals in the presence of dielectric losses

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We study defect states in two- and three-dimensional dielectric photonic crystals. We use the transfer-matrix method and we calculate the transmission and reflection coefficient of electromagnetic waves. The Q factor of the defect states increases exponentially with the thickness of the photonic crystal. However, it saturates at high thickness when absorption is introduced. The higher the absorption, the lower the saturated value of the Q factor. [S0163-1829(98)00907-2]

I. INTRODUCTION

It is now well known that the propagation of electromagnetic (EM) waves in periodic dielectric arrays can be completely forbidden for a certain range of frequencies, the so-called photonic band gap (PBG).[1] These two-dimensional (2D) or (3D) photonic crystals offer the potential to engineer the properties of the EM waves in these structures.[1] The initial interest in this subject came from the proposal to use PBG crystals to inhibit spontaneous emission in photonic devices, leading to more efficient light emitters like thresholdless semiconductor lasers and single mode light-emitting diodes.[2–5] However, the difficulties of fabricating smaller scale structures restricted the experimental demonstration of the photonic crystals to the microwave and the millimeter wave frequency regions.[6–10] There are several applications of the photonic crystals in those frequency regions such as efficient antennas, filters, sources, and waveguides.[11–18] Some of those applications are based on the presence of defect or cavity modes, which are obtained by locally disturbing the periodicity of the photonic crystal.[10,19–23] The frequencies of these modes lie within the photonic band gap, and the associated fields are localized around the defect.

In this paper, we study the properties of defect states in 2D and 3D photonic crystals. In particular, we are interested in the defect frequency, polarization, quality factor (Q), and their coupling efficiency to modes outside of the photonic crystal. We also study how these properties are affected by the introduction of the absorption.

We use the transfer-matrix method (TMM), introduced by Pendry and MacKinnon,[24] to calculate the EM transmission through a photonic crystal with defects. In the TMM, the total volume of the photonic crystal is divided in small cells and the fields in each cell are coupled with those in the neighboring cells. Then the transfer matrix can be defined by relating the incident fields on one side of the photonic crystal with the outgoing fields on the other side. Using the TMM, the band structure of an infinite periodic system can be calculated, but the main advantage of this method is the calculation of transmission and reflection properties of EM waves of various frequencies incident on a finite thickness slab of PBG material. In that case, the material is assumed to be periodic in the directions parallel to the interfaces. The TMM has previously been applied to defects in 2D PBG structures,[25] photonic crystals with complex and frequency-dependent dielectric constants,[26] metallic PBG materials,[27,28] and angular filters.[29] In all these examples, the agreement between theoretical calculations and experimental measurements was very good.

II. TWO-DIMENSIONAL CRYSTALS

We study a 2D crystal consisting of infinitely long cylinders with their axis along the z axis and forming a square lattice. The lattice constant is $a=1.27$ mm and the rods diameter 0.51 mm. We use alumina-ceramic rods with the dielectric constant 9.61. The system is finite along the y axis with thickness L. In all the cases, the electric field is parallel to the z axis. We assume periodic boundary conditions at the edges of the system in the x direction. These calculations are intended to simulate the system used by Lin *et al.* in their experiments.[23] We should point out though, that the crystal used by Lin *et al.* was finite in all the directions.

Figure 1 shows the transmission of waves traveling along the y axis (normal incidence); the thickness of the system is $L/a=11$. In the periodic case (the dotted line in Fig. 1), there is a gap between 62 and 103 GHz. This is not the full band gap since it corresponds only in the Γ-X direction in the k space. By removing the rods from the fifth and sixth layers, a peak in the transmission appears at 85.16 GHz (solid line in Fig. 1). The quality factor Q is defined as the center frequency ω_d divided by the peak's linewidth Δ at half maximum. The defect peak shown in Fig. 1 has $Q=5009$ while the transmission at the center frequency is -3 dB. That means that almost 50% of the incident power is transmitted. Also, the gap seems to increase slightly while the transmission in the middle of the gap increases with the introduction of the defect. The widening of the gap with the introduction of the defect is an interesting observation that needs further studies to be completely understood.

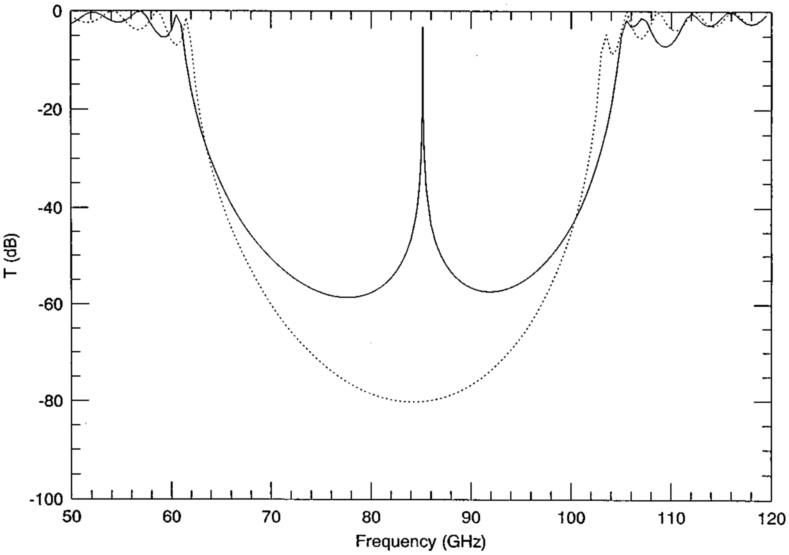

FIG. 1. The transmitted intensity (T) of EM waves propagating in a 2D square lattice consisting of cylindrical alumina rods. The lattice constant is $a=1.27$ mm, the radius of the rods is 0.255 mm, and the thickness of the system is $L/a=11$. Dotted line shows the results of a perfect lattice while the solid line corresponds to the case where two neighboring layers of rods in the middle of the structure have been removed.

Figure 2 shows the linewidth Δ of the defect peak as a function of the total thickness of the system L. In all the cases, the defect is created by removing two neighboring layers of rods in the middle of the system. The center frequency is around 85.2 GHz and the transmission at the top of the peak is -3 dB regardless of the thickness. The linewidth changes five orders of magnitude from the $L/a=5$ to 17. An exponential function (solid line in Fig. 2) fits our calculations very well, which is a general characteristic of tunneling behavior.[23] A Q value of more than 10^6 can be achieved for total thickness $L/a=17$. Our results are in good agreement with the measurements of Lin *et al.*[23] up to $L/a=14$. However, for higher L/a, they found that the linewidth saturates at a value of about 3.5 MHz. They speculate that dielectric loss should be the problem for that saturation. Indeed, the results shown in Fig. 2 support that speculation. By adding a small imaginary part in the dielectric constant ϵ, the linewidth saturates to a constant value depending on the imaginary part of ϵ. The saturated value is 0.02 and 0.1 GHz for the imaginary part of ϵ 0.01 and 0.05, respectively. We should also mention that the transmission at the top of the peak decreases by increasing the imaginary part of ϵ. In a crystal with $L/a=11$, the transmission at the top of the peak is -3, -10, and -20 dB for the imaginary part of ϵ, 0, 0.01, and 0.05, respectively.

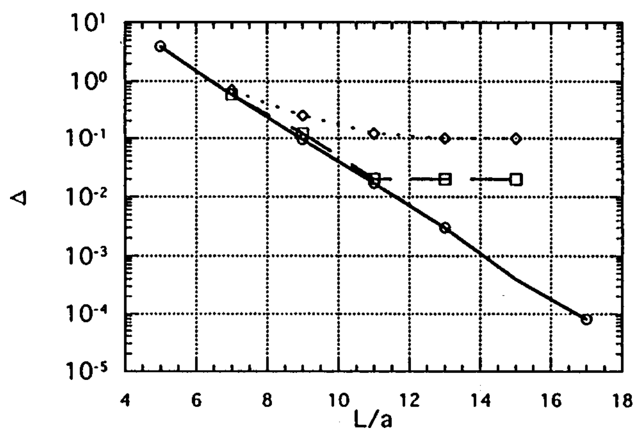

FIG. 2. The linewidth of the defect peak Δ as a function of the total thickness of the system, L/a, for imaginary part of ϵ equal to 0, 0.01, and 0.05 (solid, dashed, and dotted lines, respectively).

In order to better understand the effect of the absorption on the properties of the defect states, we show in Fig. 3 the transmission, reflection, and absorption at the top of the defect peak as a function of the imaginary part of the ϵ. The system is similar to the one in Figs. 1 and 2; results for $L/a=11$ and 9 (solid and dotted lines) are shown in Fig. 3. For a constant imaginary part of ϵ, the transmission becomes smaller as the thickness of the system increases. The transmission decreases monotonically by increasing the imaginary part of ϵ. However, the absorption has a maximum at the same value of the imaginary part of ϵ where the reflection has a minimum. The reflection at the minimum has a more than -20 dB drop. It is interesting to analyze the behavior of the absorption. The overall trend is an increase of the absorption as the imaginary part of ϵ increases. We believe that the absorption peak shown in Fig. 3(b) is due to the inhomogeneity of the structure. Although most of the wave is localized in the air defect, there is some part that is located in the absorbing cylinders.[18,30] At the peak of the absorption, the part of the wave located in the absorbing cylinders should be maximum. By increasing the thickness of the system, the maximum of the absorption (or the minimum of the reflection) appears in smaller values of the imaginary part of ϵ. So, for a particular real and imaginary part of the dielectric constant, we can adjust the thickness of our system in order to get the maximum absorption and the minimum reflection. This effect might have some applications in the construction of antireflection coatings. We expect that defect states in 3D photonic crystals will have similar dependence on the absorption.

We now study a system consisting of $L/a=11$ layers of

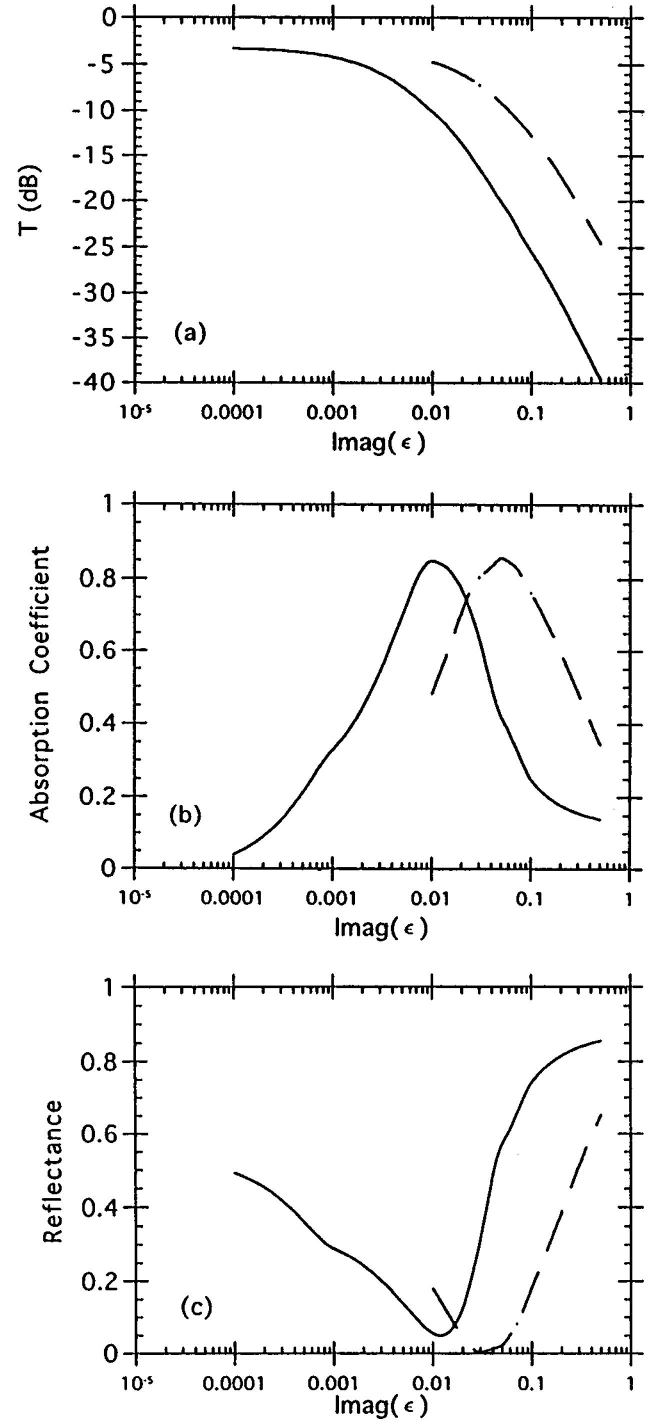

FIG. 3. The transmitted intensity T, absorption A, and reflection R, at the top of the defect peak as a function of the imaginary part of ϵ for thickness $L/a=11$ and 9 (solid and dotted lines, respectively).

rods along the y axis. Along the x axis, we use a supercell with seven unit cells and we assume periodic boundary conditions at the edges of the supercell. The defect is introduced by removing rods from the sixth layer. Figure 4 shows the defect frequency and the linewidth as a function of the cavity size. The cavity size is $(1\times m)a^2$ where m is the number of the removed cylinders. The dependence of the defect frequency from the cavity size is similar to the one measured by Lin *et al.*[23] They explained this behavior using a 2D resona-

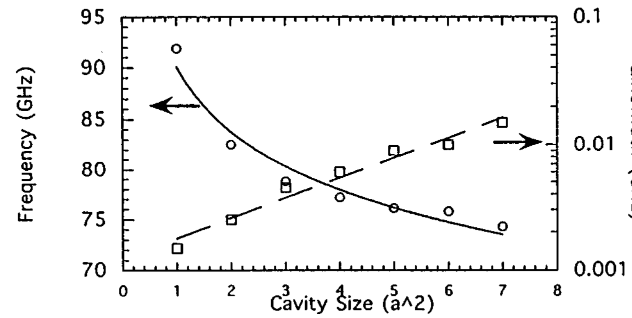

FIG. 4. Linewidth and the frequency of the defect state as a function of the cavity size.

tor model. In this model, the defect frequency is proportional to $k_x^2+k_y^2$, where $k_i=\pi/d_i$ $(i=x,y)$ are the wave vectors for the standing wave; d_x and d_y are the size of the cavity that they have been able to find by fitting this formula to their measurements. The linewidth data can be fitted very well to an exponential function, which means that the linewidth decreases exponentially by decreasing the cavity size. This is also in good agreement with the measurements reported by Lin *et al.*[23] except for cavity sizes 1 and 2. For these two sizes, they found the same linewidth in contrast with our calculations (Fig. 4). We attribute this difference to the saturation of the measured linewidth due to the absorption.

We can also tune the defect frequency along the photonic band gap by changing the radius of one of the rods.[19] Figure 5 shows the defect frequency and the linewidth of EM waves with k vector along the y axis. The thickness of the photonic crystal is $L/a=7$. In the lateral dimension (x direction), we use a supercell consisting of seven unit cells with periodic boundary conditions at the edges of the supercell. The defect is introduced by changing the radius, r_d, of one rod at the fifth layer. The radius of the undistorted rods is r. The defect state first appears for r_d/r less than 0.85 and moves along the gap from the lower edge of the gap towards the higher edge of the gap as r_d/r decreases. At $r_d/r=0$, the defect frequency is 92 GHz. The present results are in agreement with those shown in Fig. 1 of Villeneuve, Fan, and Joannopoulos.[22] The linewidth starts from relatively high values (0.105 GHz at $r_d/r=0.8$), it reaches its lowest value close to the center of the PBG (0.0205 GHz at $r_d/r=0.6$),

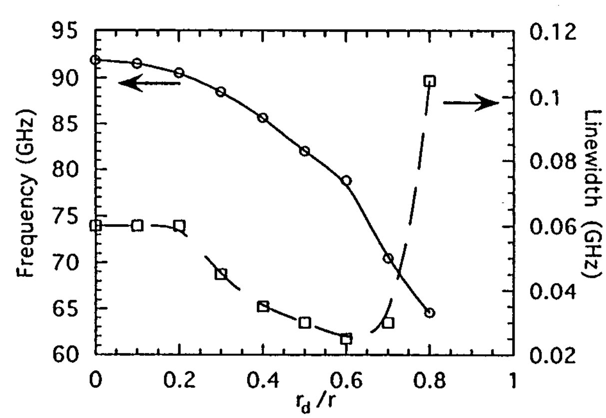

FIG. 5. Linewidth and the frequency of the defect state as a function of the ratio of the radius of the distorted rod r_d over the radius of the undistorted rod r.

and it saturates (0.06 GHz) for r_d/r tending to zero. The minimum of the linewidth in the middle of the PBG can be explained from the fact that the transmission at the center of the gap becomes minimum (dotted line in Fig. 1). So, the photonic crystal that is around the defect will be a better reflector for frequencies in the middle of the gap and that will force the wave to become more localized around the defect at these frequencies. For that reason, the linewidth has a minimum at the center of the gap. For r_d/r close to zero, the defect frequency is almost constant; for that reason the linewidth is almost the same for r_d/r less than 0.2.

III. THREE-DIMENSIONAL CRYSTALS

In this section, we study the 3D, layer-by-layer photonic crystals introduced by the Iowa State University group.[7–9,31] The structure is made of layers of cylindrical alumina rods with a stacking sequence that repeats itself every four layers with repeat distance $c = 1.272$ cm. Within each layer, the rods are arranged with their axes parallel and separated by a distance $a = 1.123$ cm. The orientations of the axes are rotated by 90° between adjacent layers. To obtain the periodicity of four layers in the direction of stacking, the rods of the second neighbor layers are shifted by a distance of $a/2$ in the direction perpendicular to the rods' axes.[7–9,31] In order to simulate this structure with the TMM, we divide the unit cell into $7\times7\times8$ subcells assuming that the z axis is along the stacking direction.

Figure 6 shows the transmission of EM waves incident on a layer-by-layer photonic crystal with four unit-cell thickness (16 layers of rods). The k vector of the incident wave is along the stacking direction (z axis). For the periodic case (dotted lines in Fig. 6), there is a gap between 11 and 15.7 GHz for both polarizations. We introduce a defect in this structure by removing every other rod in the eighth layer. A defect peak appears at 12.58 GHz. The width of the peak (0.016 GHz) is almost the same for both polarizations, and the transmission at the top of the peak (-3.4 and -29.7 dB) is higher for the polarization where the incident electric field is parallel to the axis of the removed rods. In general, the transmission for the parallel polarized waves is more affected by the defect than the perpendicular polarized waves. We can probably explain that by making the following simplification. Let us assume that the layer-by-layer structure consists of two different 2D photonic crystals. The first one has cylinders parallel to the x axis and the second one has cylinders parallel to the y axis. By creating a defect in the second 2D photonic crystal and assuming no interactions between the two polarized waves (which is a really rough approximation), we expect that only the wave with the E field parallel to the y axis will be affected by the defect. This is actually what we see in Fig. 6(b). Of course, since there is not a complete separation between the two polarizations, we also see smaller effects of the defect in the other polarization [Fig. 6(a)]. The Q factor and the defect frequency are in very good agreement with measurements in the same configuration.[20] However, the measured transmission at the top of the peak is about 10 dB smaller than the calculated one, most probably due to some small absorption of the alumina rods.[20] By increasing the thickness to eight unit cells (32 layers of rods), the width of the peak becomes 9 $\times10^{-6}$ GHz, which corresponds to Q greater than 10^6, while the defect frequency and the transmission at the top of the peak remain almost the same (12.61 GHz and -3.8 dB, respectively).

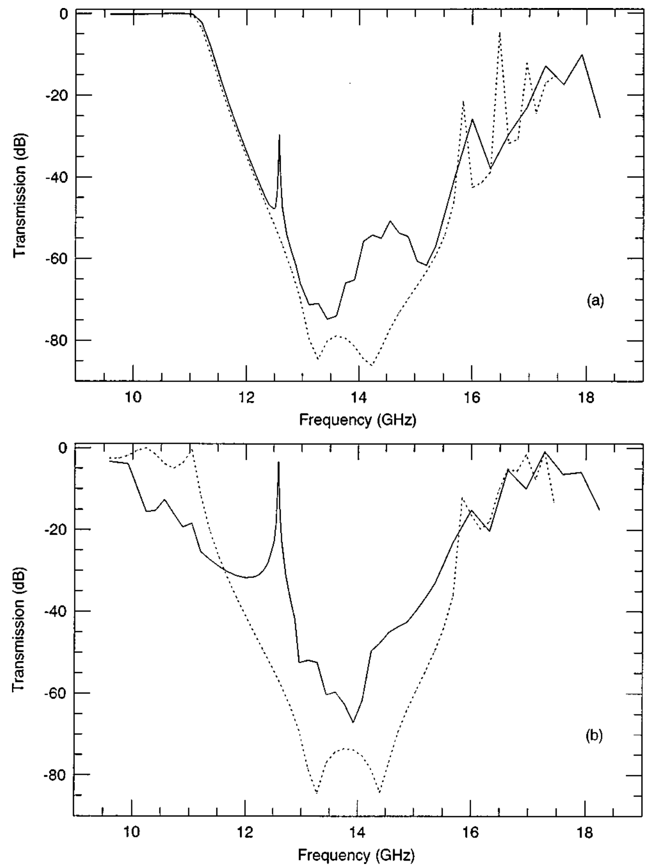

FIG. 6. The transmitted intensity of EM waves propagating through a 3D layer-by-layer PBG consisting of 16 layers of rods. The dotted line corresponds to the periodic case, while the solid line correspond to the defect case in which every other rod from the eighth layer has been removed. Panels (a) and (b) correspond to the polarization with the electric field parallel and perpendicular to the first layer of rods.

Figure 7 shows the results for a similar system with four unit-cell thickness. The defect is introduced by changing the radius of every other rod in the eighth layer. The radius of

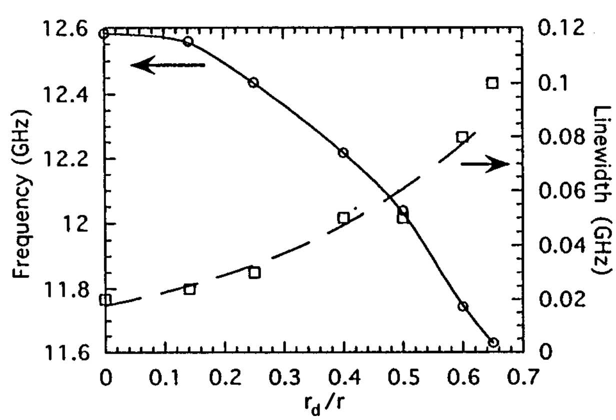

FIG. 7. Linewidth and the frequency of the defect state as a function of the ratio r_d/r.

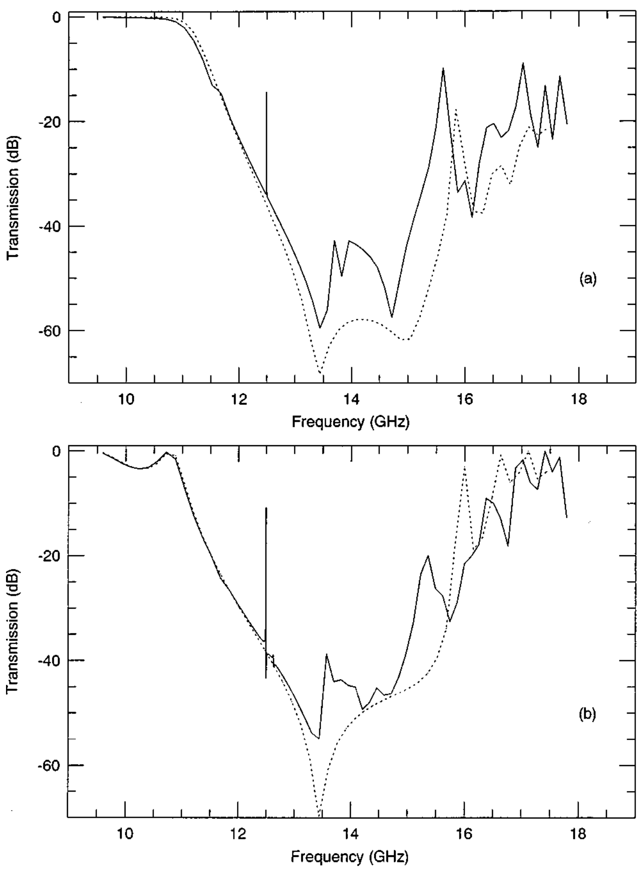

FIG. 8. The transmitted intensity of EM waves propagating through a 3D layer-by-layer PBG consisting of 12 layers of rods. The dotted line corresponds to the periodic case while the solid line corresponds to the defect case in which an additional rod has been placed after every other rod of the fifth layer. Panels (a) and (b) correspond to the polarization with the electric field parallel and perpendicular to the first layer of rods.

the defect rod is r_d, while the undistorted radius is r. The defect peak emerges from the lower edge of the gap (11 GHz) for ratios r_d/r around 0.7, and it tends to higher frequencies as r_d/r decreases. For r_d/r close to zero it saturates to the frequency of 12.6 GHz. The linewidth is 0.1 for $r_d/r=0.65$, and decreases rapidly to 0.02 GHz at $r_d/r=0$. So, we can change the position of the defect peak by changing the radius of the distorted cylinders.

We also study a case where we add extra rods. We use a similar layer-by-layer structure with three unit-cell thickness. An extra rod has been inserted after every other rod of the fifth layer of the photonic crystal. The extra rods have been placed halfway between the lattice rods. Figure 8 shows the transmission for waves traveling along the z axis and incident on the photonic crystal mentioned earlier. There is a very sharp peak for both polarizations at 12.49 GHz. The width of the peak is about 3×10^{-4} corresponding to $Q=43\,000$ for both polarizations. The transmission at the top of the peak is 4 dB higher for the polarization with the E field parallel to the added rods. Comparing the defect cases with added and removed rods, we find that in the added defects case, the results for both polarizations are similar [see Figs. 8(a) and 8(b)] in contrast with the removed defects case where the two polarizations have significant differences [see Figs. 6(a) and 6(b)]. There is no apparent explanation for that difference. We also find that the Q factors are much higher for the added rods case, while the transmission at the top of the peak is higher for the removed rods case.

IV. CONCLUSION

We have studied defect states in 2D and 3D dielectric photonic crystals. In all the cases, the calculated defect frequencies are in good agreement with the experimental measurements.[20,23] However, there are some differences between the present calculations and the measurements,[23] especially for high thickness photonic crystals. We attributed these differences to the absorption losses. In particular, we found that the linewidth of the defect states decreases exponentially with the thickness of the photonic crystal in the absence of absorption. However, it saturates at high thicknesses when we introduced absorption. The higher the absorption, the higher the saturated value of the linewidth. This explains why the measured values of the Q factor (which is inversely proportional to the linewidth) are less than several thousands.

For constant thickness, the transmission at the maximum of the defect peak decreases rapidly as the imaginary part of the dielectric constant increases. However, the reflection at the defect frequency as a function of the imaginary part of the dielectric constant, Im(ϵ), has a minimum at a particular value of Im(ϵ) that depends on the thickness of the photonic crystal. Interestingly, the reflection could be as low as -20 dB at this minimum. We argue that this effect can be used for the fabrication of efficient antireflecting coatings.

We also found that the defect frequency can be tuned along the photonic band gap by changing either the cavity size or the radius of the distorted rods in accordance with previous studies.[19,23]

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[1] Development and Applications of Materials Exhibiting Photonic Band Gaps, special issue of J. Opt. Soc. Am. B **10**, 208–408 (1993). Also, see *Photonic Band Gaps and Localization*, Proceedings of the NATO ARW, edited by C. M. Soukoulis (Plenum, New York, 1993). For a more recent review, see the articles in *Photonic Band Gap Materials*, edited by C. M. Soukoulis (Kluwer, Dordrecht, 1996).

[2] E. Yablonovitch, Phys. Rev. Lett. **58**, 2059 (1987).

[3] D. L. Bullock, C. C. Shih, and R. S. Margulies, J. Opt. Soc. Am. B **10**, 399 (1993).

[4] P. L. Gourley, J. R. Wendt, G. A. Vawter, T. M. Brennan, and B. E. Hammons, Appl. Phys. Lett. **6**, 687 (1994).
[5] J. P. Dowling, M. Scalora, M. J. Bloomer, and C. M. Bowden, J. Appl. Phys. **75**, 1896 (1994).
[6] E. Yablonovitch, T. J. Gmitter, and K. M. Leung, Phys. Rev. Lett. **67**, 2295 (1991).
[7] E. Ozbay, A. Abeyta, G. Tuttle, M. Tringides, R. Biswas, C. Soukoulis, C. T. Chan, and K. M. Ho, Phys. Rev. B **50**, 1945 (1994).
[8] E. Ozbay, E. Michel, G. Tuttle, M. Sigalas, R. Biswas, and K. M. Ho, Appl. Phys. Lett. **64**, 2059 (1994).
[9] E. Ozbay, G. Tuttle, M. Sigalas, R. Biswas, K. M. Ho, J. Bostak, and D. M. Bloom, Appl. Phys. Lett. **65**, 1617 (1994).
[10] S. L. McCall, P. M. Platzman, R. Dalichaouch, D. Smith, and S. Schultz, Phys. Rev. Lett. **67**, 2017 (1991).
[11] E. R. Brown, C. D. Parker, and E. Yablonovitch, J. Opt. Soc. Am. B **10**, 404 (1993).
[12] E. R. Brown, C. D. Parker, and O. B. McMahon, Appl. Phys. Lett. **64**, 3345 (1994).
[13] S. D. Cheng, R. Biswas, E. Ozbay, S. McCalmont, C. Tuttle, and K.-M. Ho, Appl. Phys. Lett. **67**, 3399 (1995).
[14] M. P. Kesler, J. G. Maloney, B. L. Shirley, and G. S. Smith, Microw. Opt. Technol. Lett. **11**, 169 (1996).
[15] M. M. Sigalas, R. Biswas, and K. M. Ho, Microw. Opt. Technol. Lett. **13**, 205 (1996).
[16] C. J. Maggiore, A. M. Clogston, G. Spalek, W. C. Sailor, and F. M. Mueller, Appl. Phys. Lett. **64**, 1451 (1994).
[17] K. Agi, L. D. Moreland, E. Schamiloglu, M. Mojahedi, K. J. Malloy, and E. R. Brown, IEEE Trans. Plasma Sci. **24**, 1067 (1996).
[18] J. D. Joannopoulos, R. D. Meade, and J. N. Winn, *Photonic Crystals* (Princeton University Press, New York, 1995).
[19] E. Yablonovitch, T. J. Gmitter, R. D. Meade, A. M. Rappe, K. D. Brommer, and J. D. Joannopoulos, Phys. Rev. Lett. **67**, 3380 (1991).
[20] E. Ozbay, G. Tuttle, M. Sigalas, C. M. Soukoulis, and K. M. Ho, Phys. Rev. B **51**, 13 961 (1995).
[21] E. Ozbay, G. Tuttle, J. S. McCalmont, M. Sigalas, R. Biswas, C. M. Soukoulis, and K. M. Ho, Appl. Phys. Lett. **67**, 1969 (1995).
[22] P. R. Villeneuve, S. Fan, and J. D. Joannopoulos, Phys. Rev. B **54**, 7837 (1996).
[23] S. Y. Lin, V. M. Hietala, S. K. Lyo, and A. Zaslavsky, Appl. Phys. Lett. **68**, 3233 (1996).
[24] J. B. Pendry and A. MacKinnon, Phys. Rev. Lett. **69**, 2772 (1992); J. B. Pendry, J. Mod. Opt. **41**, 209 (1994).
[25] M. M. Sigalas, C. M. Soukoulis, E. N. Economou, C. T. Chan, and K. M. Ho, Phys. Rev. B **48**, 14 121 (1993).
[26] M. M. Sigalas, C. M. Soukoulis, C. T. Chan, and K. M. Ho, Phys. Rev. B **49**, 11 080 (1994).
[27] M. M. Sigalas, C. T. Chan, K. M. Ho, and C. M. Soukoulis, Phys. Rev. B **52**, 11 744 (1995).
[28] J. S. McCalmont, M. M. Sigalas, G. Tuttle, K. M. Ho, and C. M. Soukoulis, Appl. Phys. Lett. **68**, 2759 (1996).
[29] M. M. Sigalas, J. S. McCalmont, K. M. Ho, and G. Tuttle, Appl. Phys. Lett. **68**, 3525 (1996).
[30] H. G. Algul, M. Khazhinsky, A. R. McGurn, and J. Kapenga, J. Phys.: Condens. Matter **7**, 447 (1995).
[31] K. M. Ho, C. T. Chan, C. M. Soukoulis, R. Biswas, and M. M. Sigalas, Solid State Commun. **89**, 413 (1994).