

# Optimizing the $Q$ value in three-dimensional metallic photonic band gap crystals

W. Y. Leung, G. Tuttle, M. M. Sigalas, R. Biswas,<sup>a)</sup> K. M. Ho,<sup>a)</sup> and C. M. Soukoulis<sup>a)</sup>  
*Microelectronics Research Center and Ames Laboratory-USDOE, Iowa State University, Ames, Iowa 50011*

(Received 7 November 1997; accepted for publication 16 July 1998)

A metallic photonic band gap crystal with different defect structures is fabricated. The structure is designed and built to operate in the 8–26 GHz frequency range. Defects with sharp peaks in the transmission are created by removing portions of the metallic rods in a single defect layer. A high quality factor ( $Q$ ) for the defect state is obtained by larger filling ratios and spatial separations between the unit cells. An optimized value of  $Q \geq 300$  is found for three unit cell metallic photonic band gap structure. The experimental observations agree very well with theoretical calculations using the transfer matrix method. © 1998 American Institute of Physics.  
[S0021-8979(98)04320-5]

## I. INTRODUCTION

Photonic band gap (PBG) crystals have emerged as novel materials in which no electromagnetic wave can propagate for all frequencies within a stop band or photonic band gap. The PBG crystal is a periodic structure composed of material with a high dielectric constant in a lower dielectric background such as air. The first photonic band gap crystal was fabricated by Yablonovitch *et al.*<sup>1</sup> by periodically drilling three sets of holes into a dielectric material and had a three-dimensional band gap between 12 and 15 GHz. However, a new robust layer-by-layer structure was later designed and developed by the Iowa State group to achieve a full three-dimensional band gap up to a frequency of 400 GHz.<sup>2,3</sup> A new direction has been to use metallic components in photonic crystals since metals are nearly perfect reflectors with low absorption at microwave or millimeter wave frequencies. However, metals become lossy at optical frequencies.

Meshes of connected metal wires exhibit a three-dimensional stop band from zero frequency up to a finite cutoff frequency ( $\nu_p$ )—behaving very similar to a waveguide. Such wire meshes with low metal filling ratio are the analogue of capacitive metal grids.<sup>4</sup> Three-dimensional metallic grids with band gaps at microwave,<sup>5–7</sup> millimeter-wave<sup>8</sup> and infrared frequencies<sup>9</sup> have recently been fabricated. In this article we demonstrate that a defect can be introduced into a metallic PBG crystal, generating a sharp defect peak with a high quality factor ( $Q$ ) in the transmission. Such MPBG crystals can be novel frequency-selective filters. The two-dimensional metallic mesh or a single unit cell has been extensively studied under the broad category of frequency-selective surfaces (FSS).<sup>10,11</sup> Such frequency-selective surfaces have found applications in microwave filters, radomes, polarizers, beam splitters, infrared mirrors, and for improving solar energy collection.<sup>12</sup> The

complementary inductive metallic patches are also FSS with a low-pass filtering properties.

In a recent study on metallic PBG crystals at 100 GHz,<sup>8</sup> defects were generated by periodically removing parts of the metal grid. In these defects, the  $Q$  factor of about 20 was obtained for the defect transmission peaks. Layer-by-layer metallic structures with defects<sup>6</sup> with high quality factors ( $Q \approx 1740$  for a 18 layer structure) and relatively high peak transmissions (80% for a 10 layer structure) were also reported at microwave frequencies. In these previous studies, only the thickness of the PBG crystal was varied to achieve high  $Q$  at the expense of the transmission intensity. In this report, we systematically investigate the other factors, such as different defect structures, filling ratios, and separations of unit cells, that can improve the  $Q$  factor and defect peak transmission intensity. Measurements are performed for a structure with three unit cells. Although, measurements are performed at microwave frequencies (8–26 GHz), the results can be scaled to higher frequencies simply by reducing the dimensions of the metallic PBG crystal.<sup>12</sup>

## II. EXPERIMENT

The metallic photonic band gap crystal is composed of a stack of square metal meshes, which are separated in the stacking direction as shown in Fig. 1. Each square metal mesh is composed of two sets of parallel 302 stainless-steel circular rods that are perpendicular to each other. This square mesh constitutes one unit cell of the photonic band gap crystal. Each unit cell consists of two layers of parallel rods with a rod to rod distance, i.e., lattice constant ( $d$ ) of 6.67 mm. These two layers of rods are spot welded together for rigidity. Care is taken to avoid warping the metal mesh during the spot welding. Meshes with three different rod radii, 0.254, 0.66, and 1.334 mm, are fabricated yielding three different filling ratios 0.01, 0.06, and 0.25. The filling ratio is defined as the volume filling fraction of metal per unit cell. However, the meshes of the 1.334 mm radius rods are soft soldered together rather than spot welded because the high power of the spot welder is needed. For the lowest filling ratio, the

<sup>a)</sup>Also at: Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011.

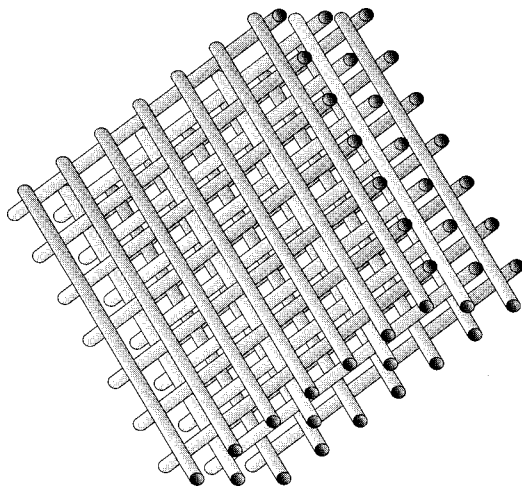


FIG. 1. Schematic diagram for the three unit cell metallic PBG crystal constructed from meshes of metallic wires. The middle unit cell shown has a defect layer with every other rod removed.

mesh always displays some degree of warping after spot welding because of the wobbly thin wires. Hence our results will concentrate on the higher filling ratios of 0.06 and 0.25. The overall size of the square mesh is 152.4 by 152.4 mm with 21 rods in the transverse directions. The resulting metallic photonic band gap crystals have cutoff frequencies of approximately 13.5, 17, and 22.5 GHz for rod radii 0.254, 0.66, and 1.334 mm, respectively, when the stacking separation between unit cells is set at 6.67 mm.

Throughout the experiment three unit cells are used for measurements unless otherwise stated. Each unit cell is separated from the other by Lexan spacers placed at four corners of the unit cell. The spacers are held together by nylon screws through alignment holes at each corner of the grid. To reduce extraneous scattering effects, no additional metal is used other than in the mesh itself. Grooves are also engraved on the spacers where the rods are positioned for lateral alignment. The resulting meshes are freely standing in the air. Two different spaces of thickness 6.67 and 9.34 mm are used. Different separations can change the transmission  $Q$  factor of the defect state as discussed later. The PBG crystal is constructed with three unit cells stacked in the  $z$  direction. The unit cell containing defects is the second unit cell placed in between the two perfect unit cells, constituting a PBG crystal with a defect.

In addition to the perfect metallic mesh, seven different defect configurations are fabricated, measured and then compared to theoretical calculations. These defects are: (A) removal of single rod, (B) removal of a complete layer of rods, (C) removal of every alternate rod in a layer, (D) removal of one of every three rods in a layer, (E) removal of one of every four rods in a layer, (F) removal of a small section of rod with a length of a lattice constant, and (G) removal of a section of wire with a length of five lattice constants. All these defects are created on one layer in the second unit cell. The defects (F) and (G) are near the center of the grid, to avoid edge effects. All measurements are performed within an anechoic chamber with two Narda horn antennas acting as transmitter and receiver. The input and output of these an-

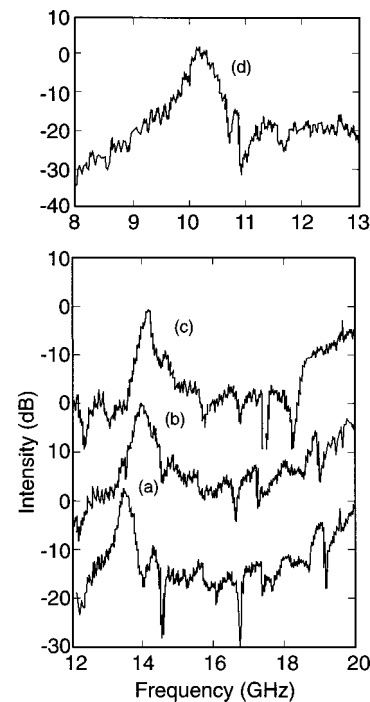


FIG. 2. Measured transmission intensity for different defects in the middle layer of the three-layer PBG crystal. (a) Every alternate rod is removed. (b) One of every three rods is removed. (c) One of every four rods is removed. (d) A complete layer is removed.

tennas are fed to a HP 8510 network analyzer. Transmission measurements only are performed on these crystals. The separation of the horns is set at a distance of  $\approx 87$  cm. The PBG crystal is placed as close as possible to the receiving horn to minimize extraneous scattering from the edge of the crystal itself. The metallic PBG crystal is typically placed a few millimeters from the receiving horn antenna.

### III. RESULTS AND DISCUSSIONS

We examined three different factors affecting the  $Q$  factor of the defect in the PBG crystal: different type of the defect, filling ratio, and the separation between two adjacent unit cells. We systematically study how the defect  $Q$  value can be affected by each of these three factors for the configuration of three unit cells. Figures 2 and 3 show the transmission measurements for the defect structures (A)–(D) and their corresponding  $Q$  factors are listed in Table I. We use the structure with a filling ratio of 0.06 and with the stacking separation among unit cells equal to the lattice constant ( $d$ ) of the mesh. Generally, all the defect peaks have  $Q \approx 60$ . Although some defects appear to have a larger  $Q$  value, they are within the experimental uncertainty. Figure 3 shows the transmission intensity for a sequence of defects starting from removal of a portion of a rod [defect F, Fig. 3(a)], to the larger section of length  $5d$  [defect G, Fig. 3(b)] and removal of a complete rod [defect A, Fig. 3(c)]. As evident in Fig. 3, no defect state is observed for the smallest defect [Fig. 3(a) or defect F]. However, as the size of defect increases, the defect transmission peak emerges and has large transmission when a complete rod is removed [Fig. 3(c)]. When the spatial size of defect is much smaller than the wavelength (2.14

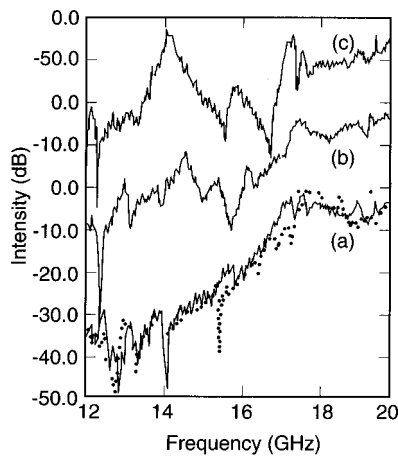


FIG. 3. Measure transmission intensity of different defects for (a) a vacancy of length  $d$  (lattice constant) i.e., defect F, (b) a vacancy of length  $5d$  (defect G), (c) one rod removed, i.e., defect A. Dotted line in (a) is the transmission for three perfect PBG unit cells.

cm for the frequency of 14 GHz), which is the case for defect (F), the perturbation to overall scattering is minimum. Hence, no defect state is observed. In fact, the transmission is very similar to a perfect PBG crystal with three unit cells. However, as the size of the defect increases, the perturbation becomes significant and its defect state becomes visible in the transmission measurement.

Another very interesting feature, shown in Fig. 2, is that the defect state has a transmission intensity larger than 0 dB, for the defect configurations B where a complete layer is removed [Fig. 2(d)] or defect C where every other rod on the same layer is removed [Fig. 2(a)]. Such a feature persists even when the whole photonic band gap crystal is moved more than one wavelength distance from the receiving antenna although there is a slight decrease of transmission intensity from the values in Fig. 2. The nature of such enhancement that may have important implications is not fully understood, although our measurements indicate it may be a finite size effect. Measurements find enhancements only for defects (B) and (C) for a filling factor of 0.06. No enhancement is observed for other filling ratios. For a filling ratio of 0.25, it is expected that the high metal content will scatter most of the incoming signal and hence reduce the transmission intensity. On the other hand, the warping of the mesh at the lowest filling ratio of 0.01 and the low defect  $Q$  for this filling ratio, may have eliminated any enhancement. It is also possible that such enhancement may be due to a focusing effect. Such focusing effects have also been investigated in a two-dimensional FSS structure<sup>13</sup> and  $\approx 5$  dB increase of transmission was observed. In order to understand the cause

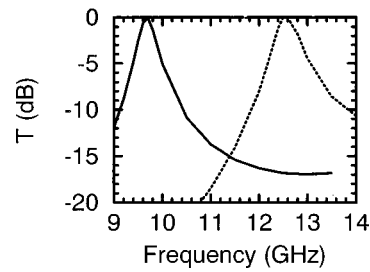


FIG. 4. Calculated transmission for a complete layer removed (solid) i.e., defect B and every alternate rod removed, i.e., defect C (dotted). The filling ratio is 0.06.

of this enhancement, a PBG crystal with twice the lateral size and with the defect (C) is fabricated. However, no signal enhancement on the defect state is observed for this larger PBG crystal. This suggests that the enhancement may be due to the finite size of the crystal.

The well-established transfer matrix method (TMM)<sup>14</sup> has been utilized for the calculation of the transmission. Figure 4 shows the calculated value of the transmission for the cases where a complete layer has been removed (defect B) and for every alternate rod removed (defect C). In both cases, the defect resides in the second unit cell, similar to experiment. The grid used in the computation is finite in the direction perpendicular to the metallic layers and has a thickness of three unit cells. However, we use periodic boundary conditions along the other two directions resulting in the metallic layers that are infinite in the lateral directions, in contrast with the experiment. Each cubic unit cell is divided into 10 by 10 by 10 subcells. Calculations with more subcells show the error in the defect frequency is less than 6%. The defect mode appears at 9.7 and 12.6 GHz for the defects B and C, respectively (Fig. 4). This is in good agreement with the experiment after accounting for the numerical errors.

Figure 5 shows the effect of filling ratio on the measured  $Q$  value of defect state. Only defect C where every alternate rod removed are shown. The other defect structures show similar trends when the filling ratio is changed. The  $Q$  value increases as the filling ratio increases. When the filling ratio is 0.25, the  $Q$  factor is about 194. However, there is a tradeoff in the reduction of the transmission intensity as the  $Q$  increases for increasing filling ratio. At high filling ratio, the defect transmission reduces to about  $-6$  dB, which may not be that desirable for frequency-selective filtering applications. This reduction is anticipated because more metal will reflect or absorb the electromagnetic waves traversing through the crystal. Calculated transmission of defects as a function of the filling ratio (Fig. 6) also predicts an enhance-

TABLE I.  $Q$  factors of three unit cells metallic photonic band gap crystal. The defect layer is placed at the second unit cell of the crystal.

Defects	Single rod removed	One layer removed	One every two rods removed	One every three rods removed	One every four rods removed	Small hole	Medium hole
$Q$ factor	$58 \pm 10$	$52 \pm 10$	$60 \pm 10$	$45 \pm 10$	$84 \pm 10$	N/A <sup>a</sup>	$70 \pm 10$

<sup>a</sup>Transmission too weak to measure.

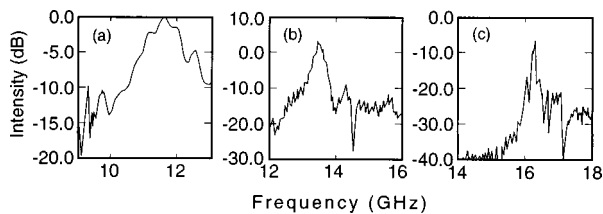


FIG. 5. Measured transmission intensity for a filling ratio of (a) 0.01, filling ratio of (b) 0.06, and filling ratio of (c) 0.25, for the defect where every alternate rod is removed, i.e., defect C.

ment of  $Q$  factor at higher filling ratio. Also, in agreement with the measurements, the calculated frequency of the defect mode decreases as the filling ratio decreases.

The calculated  $Q$  factor is generally somewhat higher than the experimental measurements. This discrepancy may be due to the finite size of the PBG crystal used in the experiment compared with the infinitely large crystal in the lateral direction used in the calculations. A PBG crystal with a smaller lateral size and the same type of defect is fabricated to test this finite size effect. The resulting measurements show a broadening of the defect peak with a slight shift of peak frequency. Overall, the experimental observations agree quite well with the theoretical calculations for the defect frequency and the  $Q$  value. However, the theoretical calculations do not predict any increase of transmission for two types of defects (B) and (C) measured above. This indicates that this effect is related to the finite size of the photonic crystal utilized in the experiment.

The last variable that may affect the  $Q$  value of the defect is the separation between unit cells. Two different separations are used in the experiment: one is the lattice constant and the other is a factor of 1.4 larger than the lattice constant. The defect structure where every alternate rod is removed (defect C) is used. As shown in Fig. 7, the  $Q$  factor increases as the separation increases. The  $Q$  values increase from about 50 for a separation factor of 1 to about 100 for the separation factor of 1.4. Such an increase is observed for other defect structures as well although not by the same factor. Such an increase of  $Q$  factor is also predicted by the TMM calculations. Figure 8 shows calculated results for a similar defect with every other rod removed in a layer with filling ratio of 0.06. The quality factor  $Q$  is 21, 71, and 187 for separation factors of 1, 1.4, and 1.8 times the lattice constant respec-

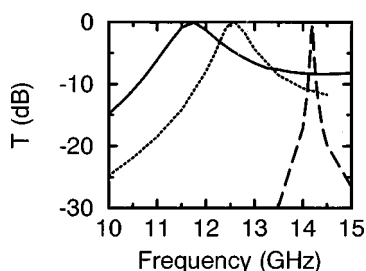


FIG. 6. Calculated transmission for every alternate rod removed, i.e., defect C. The filling ratios are 0.06, 0.12, 0.18 (solid, dotted and dashed lines, respectively).

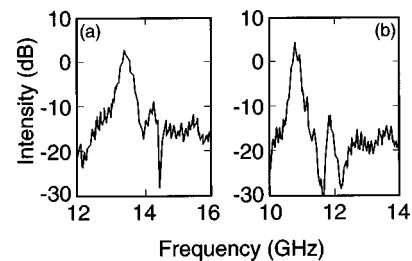


FIG. 7. Measured transmission intensity for separation between unit cells (a) equal to the lattice spacing, and (b) a factor of 1.4 larger than the lattice spacing.

tively. Also in agreement with the measurements, the calculated frequency of the defect mode decreases as the separation factor increases.

By increasing both the filling ratio and increasing the separation of unit cells we may further increase the  $Q$  value. In fact, for the defect of every alternate rod removed (defect C), we measure a  $Q$  of 350 when both of these two factors are varied together. However, the  $Q$  factor can also be increased by increasing the thickness of the PBG crystal, which has been observed experimentally and also suggested by theoretical calculations.<sup>6</sup> One serious disadvantage of increasing the thickness of the crystal has been the reduced transmission intensity of the defect peak. In this report, we explore other factors, other than the thickness of the PBG crystal, to get a better understanding of how to obtain a higher  $Q$  value. As a result of this study, higher  $Q$  can be accomplished by increasing the filling ratio and wider separation of unit cells together.

#### IV. CONCLUSION

In this study, we have demonstrated how the defect structure, filling ratio and stacking separation between unit cells can affect the  $Q$  factor of the defect. Filling ratio and stacking separation have the largest impact on the  $Q$  factor whereas the different types of defect structures have a relatively small effect. However, the defect frequency can be tuned with different defect structures. By combining the filling ratio and space separation we can achieve a much higher  $Q$  factor ( $>300$ ) than by varying any single variable alone.

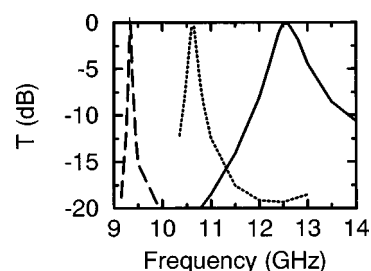


FIG. 8. Calculated transmission for every alternate rod removed. The filling ratio is 0.06. The layer separations are 1, 1.4 and 1.8 times the lattice spacing (solid, dotted, and dashed lines, respectively).

**ACKNOWLEDGMENTS**

This work is supported by the Director for Energy Research, Office of Basic Energy Sciences and Advanced Energy Projects, and the Department of Commerce through the Center of Advanced Technology (CATD). The Ames Laboratory is operated for the U.S. Department of Energy by Iowa State University under Contract No. W-7405-Eng-82.

- <sup>1</sup>E. Yablonovitch, T. J. Gmitter, and K. M. Leung, *Phys. Rev. Lett.* **67**, 2295 (1991).  
<sup>2</sup>E. Özbay, A. Abeyta, G. Tuttle, M. Tringides, R. Biswas, C. T. Chan, C. M. Soukoulis, and K. M. Ho, *Phys. Rev. B* **50**, 1945 (1994).  
<sup>3</sup>E. Özbay, E. Michel, G. Tuttle, R. Biswas, K. M. Ho, J. Bostak, and D. M. Bloom, *Opt. Lett.* **19**, 1155 (1994).  
<sup>4</sup>R. Ulrich, *Infrared Phys.* **7**, 37 (1967); V. P. Tomaselli, D. C. Edward, P. Gillan, and K. D. Möller, *Appl. Opt.* **20**, 1361 (1981); T. Timusk and P. L. Richards, *ibid.* **20**, 1355 (1981).  
<sup>5</sup>D. F. Sievenpiper, M. E. Sickmiller, and E. Yablonovitch, *Phys. Rev. Lett.* **76**, 2480 (1996).

- <sup>6</sup>E. Özbay, B. Temelkuran, M. Sigalas, G. Tuttle, C. M. Soukoulis, and K.-M. Ho, *Appl. Phys. Lett.* **69**, 3797 (1996).  
<sup>7</sup>M. Stoytchev and A. Z. Genack, *Phys. Rev. B* **55**, 8617 (1997).  
<sup>8</sup>J. S. McCalmont, M. Sigalas, G. Tuttle, K. M. Ho, and C. M. Soukoulis, *Appl. Phys. Lett.* **68**, 2759 (1996).  
<sup>9</sup>K. A. McIntosh, L. J. Mahoney, K. M. Molvar, O. B. McMahon, S. Verghese, M. Rothschild, and E. R. Brown, *Appl. Phys. Lett.* **70**, 2937 (1997).  
<sup>10</sup>*Frequency Selective Surface and Grid Array*, edited by T. K. Wu (Wiley, New York, 1995).  
<sup>11</sup>D. R. Smith, S. Shultz, N. Kroll, M. Sigalas, K. M. Ho, and C. M. Soukoulis, *Appl. Phys. Lett.* **65**, 645 (1994).  
<sup>12</sup>See review articles in *J. Opt. Soc. Am. B* **10**, 280 (1993); See also the articles in *Photonic Band Gap Materials*, edited by C. M. Soukoulis (Kluwer, Dordrecht, 1996).  
<sup>13</sup>S. Chandran and J. C. Vardaxoglou, *Microwave Opt. Technol. Lett.* **11**, 277 (1996).  
<sup>14</sup>J. B. Pendry and A. MacKinnon, *Phys. Rev. Lett.* **69**, 2772 (1992); J. B. Pendry, *J. Mod. Opt.* **41**, 209 (1994).