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Effect of point defects on band-gap properties in diamond structure photonic crystals

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Three dimensional diamond structure photonic crystals (PCs) with point defects fabricated by rapid prototyping and gel casting with alumina were studied at microwave frequencies. The sphere, ellipsoid, and cylinder point defects were introduced in the PCs first and it was found that the localization of electromagnetic wave is the strongest in ellipsoid point defect photonic crystals. Then, the size change of the ellipsoid point defect was studied to find out the optimal size. When the size of the ellipsoid point defect is close to one unit cell, the Q factor, which represents the localization intensity of the electromagnetic wave, will be the biggest. Based on the optimal size of ellipsoid point defect, more ellipsoid point defects were introduced into one diamond PC structure. Three point defect resonant modes were found in a photonic crystal with three ellipsoid point defects and the distance between each defect was twice of the lattice constant. A guided band was observed in the forbidden band gap in a photonic crystal with five ellipsoid point defects, in which the distance between each defect was of one lattice constant. © *2012 American Institute of Physics*. [doi:10.1063/1.3679128]

I. INTRODUCTION

Recently, photonic crystals (PCs)[1,2] which are periodic arrangements structures of dielectric or metallic media[3–5] have inspired great interests of scientists for its unique electromagnetic band gap property. Various kinds of photonic crystals[6–9] have been investigated and it is well-known that the three dimensional photonic crystals with diamond structure[10–12] can generate a complete band gap in all the polarization and propagation directions of the electromagnetic wave. Most of the research efforts on the diamond structure photonic crystals are concentrated on the perfect structure to pursue the wide band gap and variety of fabrication methods.[13–17] For photonic crystals, if the periodic structure is broken or modified locally by defects, the localized resonant modes of electromagnetic wave will be created in the band gap.

The guiding and bending of electromagnetic wave through highly localized defect modes in a three dimensional woodpile PC were investigated by Bayindir *et al.*[18] A three dimensional PC, in which a cube cavity of the stage 2 Menger sponge fractal is embedded, was designed in order to localize terahertz waves more effectively.[19] Aoki's group and their collaborators[20,21] proposed an idea of coupling of quantum dots with point defects cavity in 3D PCs and the Q factor of more than 8600 was achieved by tuning the cavity mode to the mid-gap frequency of the complete photonic bandgap. Kanehira *et al.*[22] investigated the effect of the defect's shape on the formation of localized defect modes of electromagnetic wave by introducing a rectangular air cavity at the center of the diamond structure photonic crystals. However, there is few investigation concerning on the shape and the size of the defects and the coupling between the defects modes.

In this work, the influence of defect shapes and defect sizes on the transmitted microwave intensity and the coupling between the defect modes have been systematically investigated. The diamond PCs with three different point defects in the shape of cylinder, sphere, and ellipsoid were fabricated and investigated first. Then, the influence of defects size on the transmitted microwave intensity was studied. At last, several defects were introduced into one PC to study the coupling property between the defects.

II. EXPERIMENTAL PROCEDURE

The fabrication method was chosen as rapid prototyping (RP) technique together with gel casting and sintering process. First, the computer aided design (CAD) models of the PCs with inverse diamond structure expanding from the unit cell and the CAD models of boxes to accommodate the PCs inside with the size rightly matching the PCs were made by Ansoft HFSS (V11, Ansoft Corporation, Pittsburgh, USA). The PCs and the box molds were then fabricated by a RP machine (Hengtong, SPS450B, Xi'an, China) according to the designed CAD models. Second, the gel containing alumina was prepared to cast into the molds. The primary solution which is composed of C_3H_5NO and $C_7H_{10}N_2O_2$ mixed well with water was prepared and the weight percentage of the organic compound is 20 wt. %. The alumina powder was added into the primary solution and the dispersant $CH_2CHCOONa$ was gradually added in. The weight percentage of the alumina ceramic powder is 75 wt. %. A little

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amount of $NH_3 \cdot H_2O$ was dropped into the slurry to adjust the *p*H value to $9 \sim 10$. The slurry was milled for 2 h after the activator $C_6H_{12}N_6$ was added. Then, the evocator $(NH_4)_2S_2O_8$ was added into the slurry. The gel was prepared well by now. Third, after the diamond structure molds and the boxes were fabricated, the gel slurry was cast into the box to about half a volume. Then, putting the PC molds into the boxes and pressing the systems slightly, the slurry gradually permeated into the interstices of the diamond structure molds. The samples were kept still for 2 h and then evacuated under −0.09 MPa to degas. The samples were dried in air at room temperature for 24 h. In the end, the samples were sintered at 1530 °C for 4 h to obtain the ceramic PCs.

The lattice constant of the PCs was chosen as 12 mm since its band gap lies at X-band of microwave frequency range.[23] The dimension of the PCs was set as 60 mm × 60 mm × 60 mm. The radius of the sphere point defect is 5 mm. The radius of the cylinder point defect is 3 mm and the height is 12 mm. The major radius of the ellipsoid point defect is 6 mm and the ellipticity is 0.5. The sizes of the point defects vary from 0.7 to 1.3 times of the original dimension of the point defects with the interval of 0.1. For one point defect PC, the point defect lies at the center of crystals. For three point defects PC, the three defects align along the center line of the crystals with a space of twice of lattice constant between each of them. As to five point defects PC, the five defects align along the center line of the crystals with one lattice constant space between each of them.

The PCs were measured by transmission/reflection (T/R) methods using a waveguide cavity connecting with a network analyzer (HP 8720ES, Hewlett-Packard, Santa Rosa, CA) to obtain the propagation characteristic of the electromagnetic wave in the PCs to investigate the change of electromagnetic wave localization in the band gap of the PCs.

III. RESULTS AND DISCUSSIONS

Figure 1 shows the section planes of single point defect PCs samples with different point defect shapes of (a) sphere, (b) ellipsoid, and (c) cylinder. The lattice constant of the PCs is 12 mm and the aspect ratio (the radius of skeleton rod to the lattice constant) is 0.37. It can be found that the samples are fabricated very well and nearly no distortion or shrinkage is appeared, which fully exhibits the advantage of the rapid prototyping with gel casting and the sintering process in the fabrication of the photonic crystals.

Figure 2 shows the transmitted microwave intensity of the defect resonant modes of the point defects with different shapes. When the electromagnetic wave propagates in the

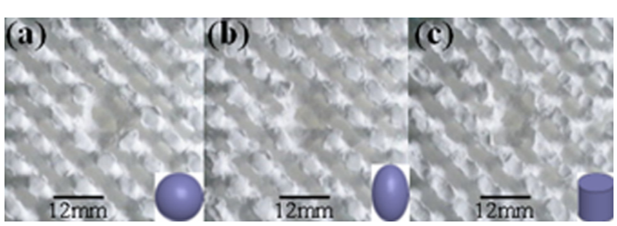

FIG. 1. (Color online) Section planes of fabricated PC samples with different point defect shapes of (a) sphere, (b) ellipsoid, and (c) cylinder.

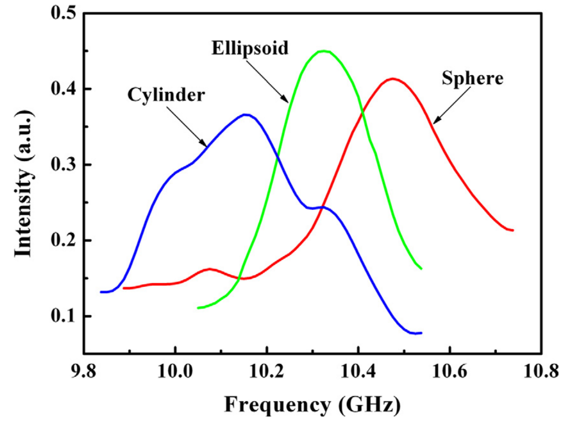

FIG. 2. (Color online) The measured transmitted microwave intensity of the defect resonant modes of point defects with different shapes.

photonic crystals with point defects, it will be locally trapped by the point defects. For the perfect PCs with diamond structure, the photonic band gap is a complete one for electromagnetic wave in any polarization and propagating directions. If the point defects are introduced into the perfect PCs, the periodical structure is broken and the point defect modes will be created in the photonic band gap when the electromagnetic wave propagates in them and which usually exhibit as resonant peaks. In Figure 2, the transmitted microwave intensities of resonant peaks excited by the three different point defects were compared. In order to compare the transmitted microwave intensities of the three different point defects more convenient, the resonant intensities have been changed into the Q factor values. The Q factor equals to the ratio of the resonant frequency and the half width of the resonant peak. The resonant peak intensities were measured from the electromagnetic wave transmission spectral of the PCs with point defects. It can be found that the Q factor, which represents the localization and the resonance of the electromagnetic wave in the defects, of the ellipsoid is the biggest and is at a value of 68. The Q factor of the sphere point defect and cylinder point defect is 42 and 27, respectively. This result indicates that the shape of point defect gives much influence on the Q factor. The theoretical formula of the Q factor is given by,[24]

$$Q = \sqrt{\frac{\mu}{\varepsilon}} \frac{2.405}{2R_S\left(1 + \frac{R}{l}\right)}, \tag{1}$$

where R_S is the surface resistance, μ is the permeability, ε is the permittivity, R is the radius of the cavity, and l is the length of the resonator cavity. If the $\frac{R}{l}$ is less, the Q value will be bigger. In the ellipsoid point defect, the $\frac{R}{l}$ is the smallest, so its Q value is the biggest. If the R tends to infinite small and the l tends to infinite big, it seems that the Q value will reach the maximum value. However, if the R is much smaller than the wavelength of the electromagnetic wave, the Q value will be probably deteriorated or the resonance will not take place. In this work, the Q value of the ellipsoid point defect is the biggest. There may be other structures that can increase the Q value further and it needs to be explored in future work.

Figure 3 shows the change of the microwave transmittance of the ellipsoid point defects with the sizes. The original size of the ellipsoid point defect in Fig. 1 is 12 mm × 6 mm× 6 mm. Then, the 0.7, 0.8, 0.9, 1.0, 1.1, 1.2, and 1.3 times of the original designed point defects were fabricated and investigated. As shown in Fig. 3, it can be found that the resonant intensity of the point defect mode created in the photonic band gap increased slightly with the size increasing and the resonant intensity reached the maximum at the original size. And the resonances of the defects decrease with the size increasing further. The biggest resonant intensity appears at the PCs with defect size near that of

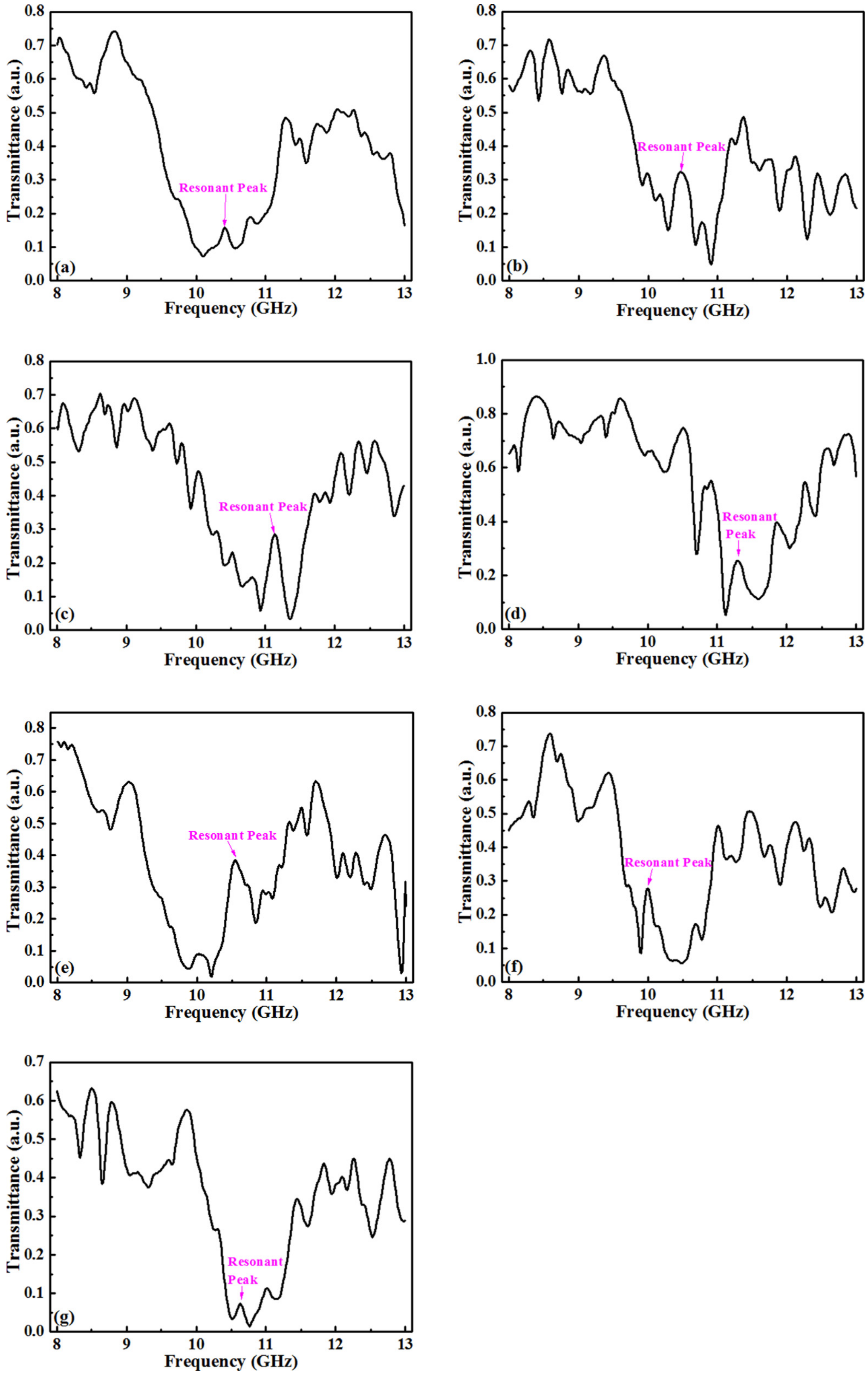

FIG. 3. (Color online) The microwave transmittance relative to the change of the sizes of ellipsoidal point defects with sizes of (a) 0.7, (b) 0.8, (c) 0.9, (d) 1.0, (e)1.1, (f) 1.2, and (g) 1.3 times of the originally designed size.

the original, the 0.9 time of the original ellipsoidal point defect size. The resonant intensity of the point defect mode with 0.9 time of the original point defect size is bigger than that in the original one, but its photonic band gap shifts to lower frequency in comparison of the perfect PC with the same structure and material parameters in Ref. 23. The photonic band gap of the PC with original size point defect matches with that of the perfect PC, thus the biggest resonant intensity is expected to appear in the point defect PC with the original size although in experimental its resonant intensity is smaller than that in the 0.9 time of the original point defect size. That is to say, when the size of the point defect is nearly the size of the original sample with 12 mm $\times$ 6 mm $\times$ 6 mm, which is one lattice constant long, the resonant intensity will be the strongest. In the point defect PCs with defect size in 0.7 and 1.3 times of the original point defect size, another resonant peak appears in the photonic band gap, but the resonant intensities of the two resonant peaks are both very small so it is of little value to verify which one is the true resonant peak. Since the resonance is induced by the localization of the electromagnetic wave in the defects, the resonant intensity will be the strongest when the point defects sizes are comparable with the wavelength of the electromagnetic wave. The design of optimal sizes is important in the design of defect PCs.

Figure 4 shows the results of the electromagnetic wave propagation in PC samples with one, three, and five point defects. The photonic band gap, the resonant peaks of the point defects, and the guiding band in the five point defects PC were marked with arrows separately. In the one point defect sample, an obvious resonant peak can be found in the forbidden band gap at 11.36 GHz. Three resonant peaks can be found in the band gap at 10.9 GHz, 11.4 GHz, and 11.7 GHz in the three point defects sample, in which the distance between the point defects is twice of the lattice constant. For the five point defects sample, in which the distance between the point defects is of one lattice constant, a guided band can be observed in the forbidden band gap from 10.89 GHz to 11.75 GHz, which exhibits a line defect property. According to Bayindir *et al.*[18] report, photons propagate through strongly localized defect cavities due to coupling between adjacent cavities modes and high transmission of electromagnetic waves (nearly 100%) is observed for various waveguide structures even if the cavities are placed along an arbitrarily shaped path. Therefore, for the five point defects sample, although the modes of each cavity are tightly confined at the defect sites, coupling between the adjacent defect modes makes the defect modes connect together to form a guide band in the forbidden band gap of the five point defects PC. In the three point defects PC, the coupling is weaker than that in the five point defects PC and so the defect modes are still independent. This result adequately indicates that the line defect property can generate in the point defects PCs by the coupling of the point defect modes.

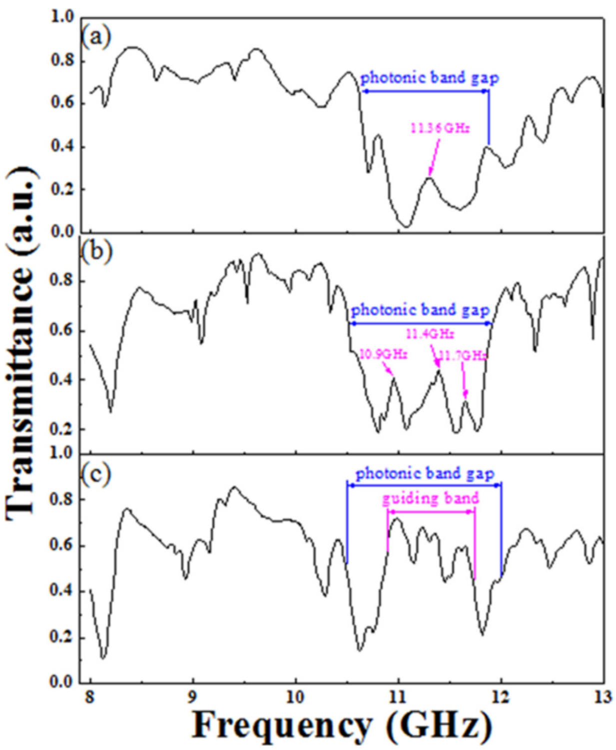

FIG. 4. (Color online) The transmission properties of electromagnetic wave in PCs with (a) one point defect in the center of the crystals, (b) three point defects aligning along the center line of the PC with two lattice constants interval between each of them, and (c) five point defects aligning along the center line of the PC with one lattice constant interval between each of them.

IV. CONCLUSIONS

In summary, the photonic crystals with point defects fabricated by rapid prototyping technique, gel casting, and sintering process were investigated. The ellipsoid point defects can localize the electromagnetic wave much more intensively comparing with the sphere and cylinder point defects. The size of the point defects will influence the resonant intensity of the electromagnetic wave in the defects. With the increasing of size of the point defects, the resonant intensity will increase and then reach the maximum value at the size of one unit cell. For the three independent point defects photonic crystals, three resonant peaks were found in the forbidden band. A guided band, which expresses a line defect property, was found in the forbidden band due to the coupling of the adjacent defect modes in the five point defects photonic crystals.

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[1]S. John, Phys. Rev. Lett. **58**, 2486 (1987).
[2]E. Yablonovitch, Phys. Rev. Lett. **58**, 2059 (1987).
[3]D. R. Smith, S. Schultz, N. Kroll, M. Sigalas, K. M. Ho, and C. M. Soukoulis, Appl. Phys. Lett. **65**, 645 (1994).
[4]M. M. Sigalas, C. T. Chan, K. M. Ho, and C. M. Soukoulis, Phys. Rev. B **52**, 11744 (1995).
[5]D. F. Sievenpiper, M. E. Sickmiller, and E. Yablonovitch, Phys. Rev. Lett. **76**, 2480 (1996).

[6]S. Y. Lin, J. G. Fleming, D. L. Hetherington, B. K. Smith, R. Biswas, K. M. Ho, M. M. Sigalas, W. Zubrzycki, S. R. Kurtz, and J. Bur, Nature **394**, 251 (1998).
[7]O. Toader and S. John, Science **292**, 1133 (2001).
[8]Y. A. Vlasov, X. Z. Bo, J. C. Sturm, and D. J. Norris, Nature **414**, 289 (2001).
[9]M. H. Qi, E. Lidorikis, P. T. Rakich, S. G. Johnson, J. D. Joannopoulos, E. P. Ippen, and H. I. Smith, Nature **429**, 538 (2004).
[10]J. D. Joannopoulos, P. R. Villeneuve, and S. H. Fan, Nature **386**, 143 (1997).
[11]K. M. Ho, C. T. Chan, and C. M. Soukoulis, Phys. Rev. Lett. **65**, 3152 (1990).
[12]J. W. Haus, J. Mod. Opt. **41**, 195 (1994).
[13]M. Miyake, Y. C. Chen, P. V. Braun, and P. Wiltzius, Adv. Mater. **21**, 3012 (2009).
[14]K. Takagi and A. Kawasaki, Appl. Phys. Lett. **94**, 021110 (2009).
[15]S. Kirihara, Y. Miyamoto, K. Takenaga, M. W. Takeda, and K. Kajiyama, Solid State Commun. **121**, 435 (2002).
[16]J. W. Galusha, M. R. Jorgensen, and M. H. Bartl, Adv. Mater. **22**, 107 (2010).
[17]K. Edagawa, S. Kanoko, and M. Notomi, Phys. Rev. Lett. **100**, 013901 (2008).
[18]M. Bayindir, B. Temelkuran, and E. Ozbay, Phys. Rev. B **61**, 18 (2000).
[19]Y. Miyamoto, H. Kanaoka, and S. Kirihara, J. Appl. Phys. **103**, 103106 (2008).
[20]K. Aoki, D. Guimard, M. Nishioka, M. Nomura, S. Iwamoto, and Y. Arakawa, Nature Photon. **2**, 688 (2009).
[21]A. Tandaechanurat, S. Ishida, K. Aoki, D. Guimard, M. Nomura, S. Iwamoto, and Y. Arakawa, Appl. Phys. Lett. **94**, 171115 (2009).
[22]S. Kanehira, S. Kirihara, and Y. Miyamoto, J. Am. Ceram. Soc. **88**(9), 2480 (2005).
[23]W. Dai, H. Wang, D. Zhou, Z. Shen, Y. Li, and D. Li, J. Am. Ceram. Soc. **93**(12), 3980 (2010).
[24]J. Fu and E. Feng, *Advanced Electromagnetic Theory* (Xi'an Jiaotong University Press, Xi'an, 2000).