Photonic Amorphous Diamond Structure with a 3D Photonic Band Gap

Keiichi Edagawa,[1] Satoshi Kanoko,[1] and Masaya Notomi[2,3]

[1]*Institute of Industrial Science, The University of Tokyo, Komaba, Meguro-ku, Tokyo 153-8505, Japan*
[2]*NTT Basic Research Laboratories, NTT Corporation, 3-1, Morinosato-Wakamiya Atsugi, Kanagawa 243-0198, Japan*
[3]*Japan Science and Technology Agency, CREST, Japan*

(Received 28 September 2007; published 2 January 2008)

We report that a full three-dimensional (3D) photonic band gap (PBG) is formed in a photonic amorphous structure in spite of complete lack of lattice periodicity. It is numerically shown that the structure ''photonic amorphous diamond'' possesses a sizable 3D PBG (18% of the center frequency for Si-air dielectric contrast) and that it can confine light at a defect as strongly as conventional photonic crystals can. These findings present important new insight into the origin of 3D PBG formation and open new possibilities in developing 3D PBG materials.

DOI: 10.1103/PhysRevLett.100.013901 PACS numbers: 42.70.Qs, 78.20.Bh

In 1987, Yablonovitch [1] and John [2] proposed the idea that a three-dimensional (3D) photonic band gap (PBG), in which electromagnetic wave propagation is forbidden in all directions, can be realized in artificial 3D periodic dielectric structures. Since then, those ''photonic crystals'' have attracted much attention and have been studied extensively because of their wide potential applications in optics. In general, PBG in photonic crystals is compared to electronic band gap in semiconductors. In many cases, the formation of PBG is explained by the Bragg scattering of photons by a periodic lattice; multiple interference effects by Bragg scattering create an energy gap along the Brillouin zone boundary. This explanation naturally requires the existence of the periodic lattice for the formation of PBG, and therefore it has been widely believed that the lattice periodicity is indispensable for the PBG formation. However, there is another explanation of the formation of band gaps, based on a viewpoint of a tight-binding model, which is frequently used in the case of electronic band gaps in semiconductors. Two electrons bound to each of the two closely located atoms can couple to form bonding and antibonding states. In solids, they form, respectively, bonding and antibonding bands, leaving an energy gap between them. This explanation does not require the lattice periodicity nor long-range order. In fact, many amorphous semiconductors, such as a-Si and a-Ge, are known to form large electronic band gaps as well as their crystalline counterparts.

The extension of the tight-binding model to photonic systems has been proposed in some 2D and 3D systems [3,4]. This would imply that PBGs can also be formed without the lattice periodicity. Indeed, in some 2D photonic amorphous structures, the PBG formations have been reported [5,6]. However, even in those 2D examples, clear PBGs are formed only for TM modes and no ''complete'' 2D PBGs (PBGs both for TM and TE modes) are realized. On the other hand, in 3D systems, which have larger directional degrees of freedom and involve vector nature of electromagnetic fields explicitly, PBG should be much more difficult to be realized; the photonic structures with 3D PBG so far found are limited to very few types of photonic crystals, and no photonic amorphous structures with 3D PBG have been reported. In this Letter, we report that the 3D PBG formation is, in actual fact, possible in a photonic amorphous structure in spite of complete lack of lattice periodicity. We also show that the photonic amorphous structure can confine light at a defect as strongly as conventional photonic crystals can.

The photonic amorphous structure we present here is a ''photonic amorphous diamond (PAD)'', which is based on a ''continuous-random-network'' (CRN) of diamondlike tetrahedral-bonding configuration originally developed as a model atomic-structure of amorphous Si or Ge [7]. For detailed design of CRN, we used the CRN structure constructed and provided by Barkema and Mousseau [8]. This CRN structure consists of a periodic arrangement of a cubic supercell with the size $(11.5d)^3$ (d: the average bond length) The supercell contains 1000 atoms. We modeled the PAD structure by connecting the tetrahedral bonds with dielectric rods in air background. For comparison, we also constructed the photonic crystalline diamond (PCD) by connecting tetrahedral bonds in the crystalline diamond structure with dielectric rods. Parts of the modeled structures are drawn in Figs. 1(a) and 1(b). We notice that the PAD consists of a network of local tetrahedral-bonding configurations, as in the PCD. However, the lattice periodicity seen in the PCD disappears completely in the PAD.

The presence of the short-range order and the absence of the long-range order in the PAD can be verified by examining the radial distribution function (RDF). Figure 2 shows the RDF calculated for the CRN structure. Here, the RDF $f(r)$ indicates the average atomic density in the spherical shell $(r, r + dr)$ around an arbitrarily selected atom, where the density is normalized to the total atomic density; when the structure has no order, $f(r)$ should be $f(r) = 1 = \text{const}$. We notice in Fig. 2 that the first peak at $r = d$ and the second peak at $r \approx 1.7d$ are clearly seen. The third and the fourth peaks are marginally observed at

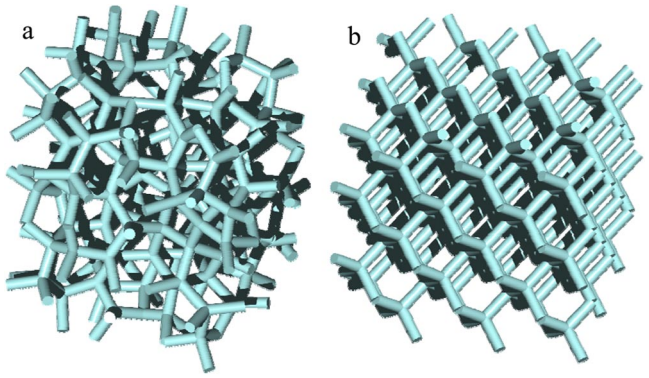

FIG. 1 (color online). 3D structures of the photonic amorphous diamond (a) and photonic crystalline diamond (b). The former was constructed from the CRN structure provided by Barkema and Mousseau [8].

$r \approx 2.4d$ and $3d$, respectively. However, no peaks can be detected in the range $r > 3.5d$, i.e., $f(r) = 1 = \text{const}$ in $r > 3.5d$. In conclusion, the RDF in Fig. 2 shows that our PAD has a definite short-range order in the range $r < 2d$ but has no long-range order in $r > 3.5d$. It should be noted that the range $r > 3.5d$ corresponds to $r > 1.5a$, where $a = 4d/\sqrt{3}$ denotes the lattice constant of the crystalline diamond. This verifies the fact that our PAD has no trace of the diamond-lattice periodicity. We confirmed this fact also by examining the diffraction pattern of the structure; the Bragg diffraction peaks completely disappear. So far, effects of disorder on PBG have been investigated in some 3D photonic crystals [9–11]. In those studies, various types of disorders (positional disorder, size disorder, stacking fault, etc.) are introduced into perfect photonic crystals but the original lattice structures are preserved on average: the Bragg diffraction peaks remain with some intensity reduction. In this point, our PAD is substantially different from those previously studied disordered 3D photonic crystals.

The photonic density of states (PDOS) for the PAD with the supercell of $(11.5d)^3$ were calculated by a finite difference time domain (FDTD) spectral method originally developed by Chan *et al.* [12]. This method is, in particular, useful for the PDOS calculations in disordered systems [13] and quasiperiodic systems [14], for which large supercells are required, because this is an order-N method. In the present study, we adopted the initial magnetic and electric fields [13], $\mathbf{H}(\mathbf{r}) = \sum_{\mathbf{G}} \mathbf{H}_{\mathbf{G}} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}+i\phi_{\mathbf{G}}}$ and $\mathbf{E}(\mathbf{r}) = \mathbf{0}$, where $\mathbf{G}$ denotes the reciprocal vector for the supercell, $\mathbf{k}$ is the Bloch wave vector, $\mathbf{H}_{\mathbf{G}}$ is a randomly chosen unit vector perpendicular to $(\mathbf{k} + \mathbf{G})$, and $\phi_{\mathbf{G}}$ is a random phase. Then, the time evolutions of $\mathbf{H}$ and $\mathbf{E}$ fields in the supercell were calculated by a FDTD method under the boundary condition of the Bloch theorem. Spectral intensities were calculated by Fourier transforming the time dependences of the fields at selected sampling points. The sum of the spectral intensities over the sampling points represents the PDOS. We calculated the spectra only for a few $\mathbf{k}$ points in the Brillouin zone and present only the spectra for $\mathbf{k} = \mathbf{0}$ [14]; when the supercell is large enough, $\{\mathbf{G}\}$ should be distributed in the reciprocal space densely enough for us to locate unambiguously the spectral gaps. For the PCD, we assumed a fictitious supercell of $(5a)^3 = (11.5d)^3$. This supercell contains 1000 "atoms" and has the same size as that of the PAD. We calculated the spectral intensity for the PCD by applying the above-described method to the fictitious supercell. This is for the purpose of comparing the spectra calculated under exactly the same conditions for the two structures. For the sampling points, we selected randomly 100 points in the cubic unit cell for the PCD and evenly distributed 1000 points in the supercell for the PAD. In all the calculations, we assumed the Si-air dielectric contrast, i.e., 13/1.

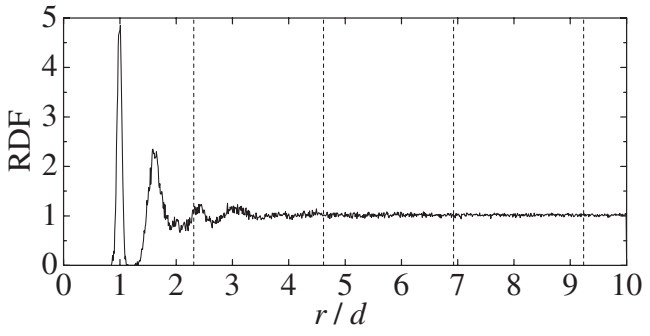

FIG. 2. Radial distribution function of the CRN structure used for the construction of the photonic amorphous diamond. Broken vertical lines indicate the positions $r = a$, $2a$, $3a$, and $4a$ (a: the lattice constant of the crystalline diamond).

Figures 3(a) and 3(b) show the spectral intensities calculated for the PAD and PCD, respectively. Here, the radius of dielectric rod is $0.26d$ and the resultant air-volume fraction is 78%. In the low frequency region below about $f = 0.15(c/d)$ (c: speed of light), the spectra have well-isolated peaks, indicating that the sampling point density in the reciprocal space is not enough. In contrast, above about $f = 0.15(c/d)$, the spectra comprise a continuous curve with spikes on them, indicating that the sampling point density is large enough for us to locate unambiguously the gaps, if any, above $f = 0.15(c/d)$. Indeed, we find clear PBGs at the frequency region around $f = 0.24(c/d)$ both for the two structures. The gap depths are also nearly the same, indicating no appreciable localized-state formations in the gap for the PAD. We have confirmed that the gap for the PAD is reproduced perfectly by the calculations for different $\mathbf{k}$ and by those using different initial fields with different random sets of $\{\mathbf{H}_{\mathbf{G}}\}$ and $\{\phi_{\mathbf{G}}\}$. The gap width to the midgap frequency ratio is 18% for the PAD and 26% for the PCD. Here, the PBG position and width for the PCD agree well with those calculated previously [12], indicating the validity of the present calculations. It should be stressed here that the supercell periodicity is not relevant to the PBG formation in the PAD; we have confirmed that a different supercell-

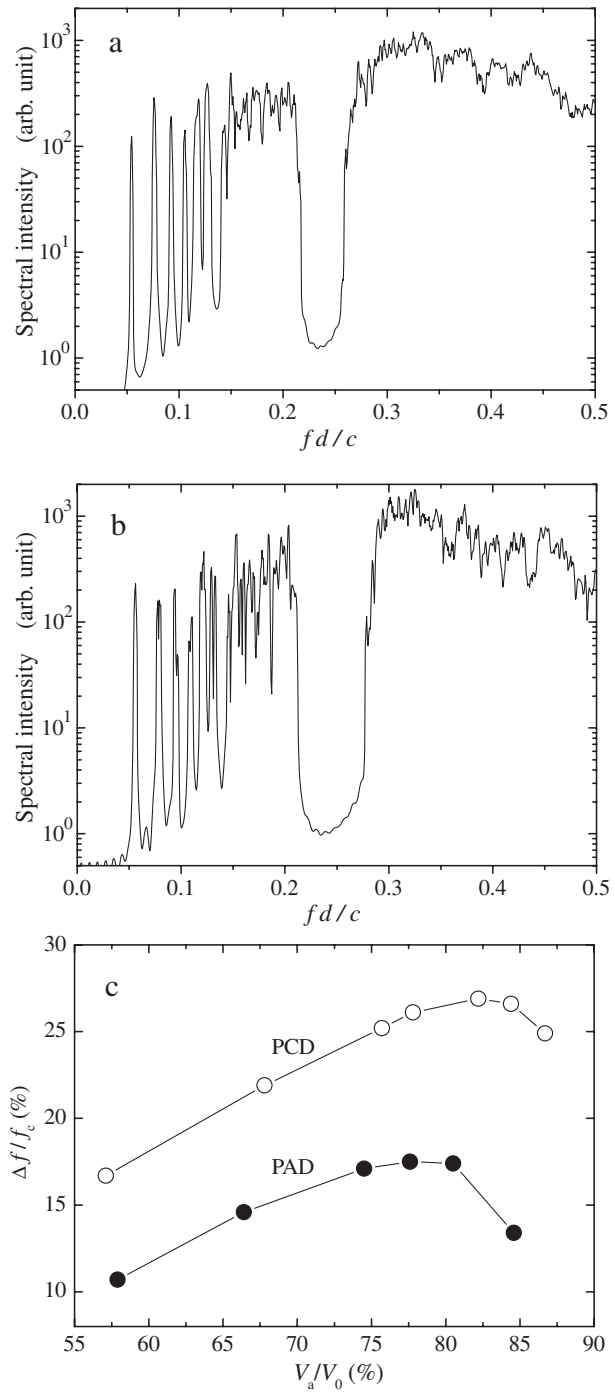

FIG. 3. Spectral intensities calculated for the photonic amorphous diamond (PAD) (a) and for the photonic crystalline diamond (PCD) (b). The air-volume fraction is $V_a/V_0 = 78\%$ for the two structures. Air-volume-fraction dependences of the gap width for the PAD and PCD (c).

size model provided by Barkema and Mousseau [8] gives the PBG exactly at the same frequency region.

Figure 3(c) shows air-volume-fraction (V_a/V_0) dependences of the gap width for the PAD and PCD. For the former, the gap width is the largest at $V_a/V_0 \approx 78\%$ while for the latter the largest gap of 27% is realized at $V_a/V_0 \approx 82\%$. It should be noted that the PCD structure here with $V_a/V_0 \approx 82\%$ is nearly the same as the champion structure that has been reported to exhibit the largest gap ever found ($\approx 30\%$) [15,16].

In realizing various types of light-controlling devices by introducing defect levels in the PBG, the capability of confining light strongly is essentially important. To see whether our PAD can do this, we have investigated by a FDTD method the attenuation behavior of an evanescent wave within the gap. Figure 4(a) shows the dependence of the field intensity (I) on the distance (r) from the surface when the electromagnetic plane wave with the gap-center frequency enters the structure. Both data show exponential decay: i.e., $I = I_0 \exp(-r/r_c)$ (r_c: the attenuation length) with nearly the same r_c ($\approx 0.6d$). This indicates that our PAD can confine light as strongly as the PCD.

In general, exponential attenuation of light transmission can also be caused by photon localization in disordered photonic crystals [2,9,10]. When disorder is introduced in a photonic crystal with PBGs, photonic states within the bands and near a band edge possibly become localized, and then exponential decay should be observed for the light with the corresponding frequency. In such a case, r_c is generally much larger than the value $r_c \approx 0.6d$ evaluated for the PAD. On the other hand, r_c for the light within the gap generally increases by the introduction of disorder due to the creation of localized states in the gap [9,10]. Nearly the same r_c for the PAD as for the PCD shown in Fig. 4(a) indicates no appreciable localized-state formations in the PBG of the PAD.

In Figs. 4(b)–4(d), the confinement of light at a defect in the PAD is demonstrated. Here, a defect is introduced by removing an arbitrarily selected dielectric rod. Figure 4(b) presents the spectral intensity at the center of the removed rod, where we can see a sharp defect peak at $f = 0.242(c/d)$ in the PBG. The mode profiles corresponding to this peak are shown in Figs. 4(c) and 4(d), where the position of the removed rod is indicated by white circle or rectangle. We can see that this mode is well confined to the defect position, as expected from the strong attenuation of evanescent wave shown in Fig. 4(a).

The photonic crystals with sizable 3D PBG so far found are all based on the crystalline diamond structure, which include Yablonovite, spiral diamond, wood pile, bcc diamond, etc., as reviewed by Maldovan and Thomas [15]. Our finding that the amorphous diamond also exhibits a sizable PBG proves that Bragg scattering by the periodic lattice is not relevant to the diamond-gap formation and the origin of the gap is in the diamondlike short-range order. With regard to the realization of large PBGs, photonic amorphous structures should have the following advantage. In the case of photonic crystals, Bragg scattering is stronger in certain crystal axes. This makes PBG anisotropic, which should limit the width of the full 3D PBG. This is the reason why crystals having more isotropic Brillouin zone are favorable for larger PBG [16]. Concerning this aspect, photonic amorphous structures are advanta-

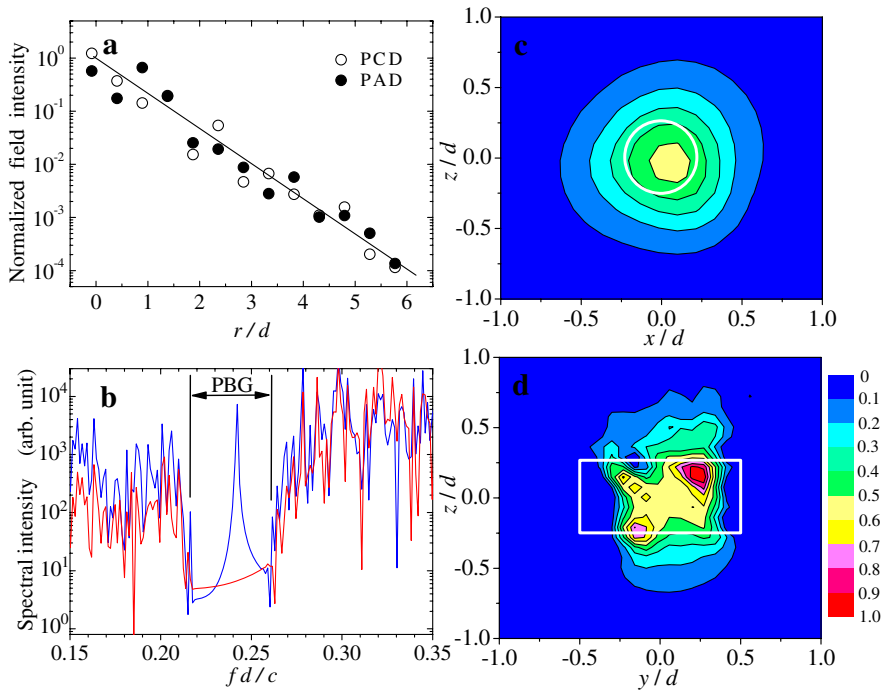

FIG. 4 (color online). (a) Attenuation behavior of the evanescent wave with the midgap frequency for the photonic amorphous diamond (PAD) and the photonic crystalline diamond (PCD), where the dependences of the incident electromagnetic wave intensity on the distance from the surface are plotted; (b) the spectral intensity at the center of the removed rod (blue) and that at the same position calculated for the perfect structure; (c) and (d) the defect mode profiles on two mutually orthogonal planes. The defect is introduced by removing a dielectric rod. The position of the missing rod is indicated by white rectangle or circle.

geous because they are completely isotropic. By tuning the structural parameters such as the degree of short-range order in the amorphous structure, we may be able to realize larger PBG than that in the champion crystalline structure.

So far, only ''photonic crystals'' have been targeted in fabricating 3D PBG materials. Our finding that photonic amorphous structures can also have 3D PBGs should open new possibilities in fabricating 3D PBG materials. For example, 3D random network structures are known to form by a new type of phase separation ''viscoelastic phase separation'' [17] in various systems such as polymer solutions, colloidal suspensions, protein solutions, etc. Some of those random networks have been shown to possess local tetrahedral-bonding configurations just like the PAD [18]. Thus, they should be strong candidates for photonic amorphous materials with 3D PBGs.

In conclusion, we presented the first amorphous structure ever found having 3D PBG in spite of complete lack of lattice periodicity. This structure, ''photonic amorphous diamond (PAD)'', exhibits a large PBG of 18% of the center frequency for Si-air dielectric contrast. The attenuation of the evanescent wave with the midgap frequency in the PAD is as strong as that in a photonic crystalline diamond. This fact indicates that the PAD can confine light strongly at a defect, which was numerically demonstrated. These findings present an important new insight into the origin of the 3D PBG formation and open new possibilities in exploring large 3D PBG structures and also in fabricating PBG materials.

We thank Professor G. T. Barkema of Utrecht University for providing the coordinates of his CRN structures and Professor T. Dotera of Kyoto University for valuable comments.

[1] E. Yablonovitch, Phys. Rev. Lett. **58**, 2059 (1987).
[2] S. John, Phys. Rev. Lett. **58**, 2486 (1987).
[3] E. Lidorikis, M. M. Sigalas, E. N. Economou, and C. M. Sokoulis, Phys. Rev. Lett. **81**, 1405 (1998).
[4] H. Miyazaki and Y. Jimba, Phys. Rev. B **62**, 7976 (2000).
[5] C. Jin, X. Meng, B. Cheng, Z. Li, and D. Zhang, Phys. Rev. B **63**, 195107 (2001).
[6] H. Miyazaki, M. Hase, H. T. Miyazaki, Y. Kurokawa, and N. Shinya, Phys. Rev. B **67**, 235109 (2003).
[7] D. E. Polk, J. Non-Cryst. Solids **5**, 365 (1971).
[8] G. T. Barkema and N. Mousseau, Phys. Rev. B **62**, 4985 (2000).
[9] Y. A. Vlasov, M. A. Kaliteevski, and V. V. Nikolaev, Phys. Rev. B **60**, 1555 (1999).
[10] V. Yannopapas, A. Modinos, and N. Stefanou, Phys. Rev. B **68**, 193205 (2003).
[11] Z. Y. Li and Z. Q. Zhang, Phys. Rev. B **62**, 1516 (2000).
[12] C. T. Chan, Q. L. Yu, and K. M. Ho, Phys. Rev. B **51**, 16 635 (1995).
[13] E. Lidorikis, M. M. Sigalas, E. N. Economou, and C. M. Soukoulis, Phys. Rev. B **61**, 13 458 (2000)
[14] Y. S. Chan, C. T. Chan, and Z. Y. Liu, Phys. Rev. Lett. **80**, 956 (1998).
[15] M. Maldovan and E. L. Thomas Nat. Mater. **3**, 593 (2004).
[16] C. T. Chan, S. Datta, K. M. Ho, and C. M. Soukoulis, Phys. Rev. B **50**, 1988 (1994).
[17] H. Tanaka, J. Phys. Condens. Matter **12**, R207 (2000).
[18] H. Tanaka and Y. Nishikawa, Phys. Rev. Lett. **95**, 078103 (2005).