Band structure of a photonic crystal with the clathrate Si-34 lattice

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The band structure of a photonic crystal with the clathrate Si-34 lattice comprising 34 lattice sites in the unit cell is studied. The structure with lattice sites connected by dielectric rods is found to have a large isotropic band gap for a wide range of permittivity. The structures composed by dielectric spheres or air spheres in dielectric have a small gap or do not possess the band gap at all, correspondingly. The relationship between the photonic band isotropy and the permittivity is deduced. The results described below make this photonic crystal very promising for potential applications.

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Photonic crystals (PhCs) are periodic structures composed of two or more materials with different permittivities that possess a complete photonic band gap (PBG).[1] If there is a complete PBG, the propagation of light is forbidden in all directions of the spectral range coincident with the band gap. The fabrication of three-dimensional (3D) macroscopic photonic crystals that have the PBG in the infrared and visible spectral range allows obtaining a number of effects that previously were beyond the observation, the most significant being a possibility to control the spontaneous emission.[2]

Since the PhC lattices have a submicron size, their fabrication calls for the development of advanced methods.[3–8] Besides, the least presently known refractive index of the lattice material that can have a complete PBG is $n=2$ for the diamond crystal lattice.[9,10] This fact significantly constrains the choice of the material because, for example, the refractive index of polymers and glasses in the visible range is normally below the said value. This problem can be addressed through the use of 3D photonic quasicrystals and periodic structures with a large number of sites ("atoms") in the unit cell. One would expect that high-degree isotropy will make it possible to reduce the PBG threshold in terms of refractive index. In the microwave range, an icosahedral photonic quasicrystal fabricated by stereolithography has been experimentally found to have large band gaps.[11] The microwave transmittance of the icosahedral photonic quasicrystal was experimentally measured. Later, photonic quasicrystals were synthesized by two-photon absorption lithography with the lattice constants, corresponding to the near infrared region.[12] Except this, quasiperiodic lattices were obtained by arrangement of microspheres by holographic optical tweezers.[13]

In spite of obvious success in synthesis of 3D photonic quasicrystals, band-structure analysis of quasicrystals was restricted mainly by two-dimensional (2D) case.[14] For band-structure calculations a plane-wave expansion technique is usually used.[15] But this method cannot be directly applied to quasicrystal because of its nonperiodic nature. To solve this problem one can use a periodic approximant of the quasicrystal and consider the tendency as the cell size becomes sufficiently large.[16,17] It was shown that for the case of 2D lattices the higher isotropy of quasiperiodic structures gives lower threshold values of dielectric contrast for gap opening.[17,18]

In 3D case photonic band gap was found in structure of icosahedral quasicrystal approximants.[19] Recently a method was presented by which the energy spectrum of a quasicrystal can be obtained by solving Maxwell's equations in higher dimensions for any quasicrystal defined by the standard cut-and-project approach.[20] This method was realized for 1D case but the theoretical analysis of the photonic band structure for 3D quasicrystals was omitted. As an alternative to photonic quasicrystals and their approximants one can consider crystals with many atoms per unit cell as a lattice of higher isotropy. In 2D case it was shown that such crystals can have wide and isotropic band gap.[21,22] In 3D case a pyrochlore crystal lattice with four atoms in the unit cell was theoretically studied.[23] The PhC was shown to have PBGs comparable in size with the diamond lattice's PBG.

Below, a PhC with a large number of per-unit-cell sites with isotropic properties is exemplified by a crystal with the clathrate Si-34 crystal lattice.[24] This lattice belongs to a class of face-centered-cubic (fcc) lattices containing 34 sites per cell (see Fig. 1). The lattice is obtained by packing a pentagonal dodecahedron and tetrakisdecahedron. In Si-34, each atom is bonded with four neighbors by distorted tetrahedral

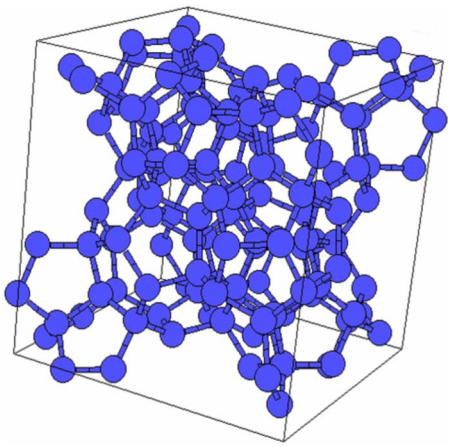

FIG. 1. (Color online) Four unit cells of the Si-34 lattice.

bonds. The diamond crystal lattice, known to have tetrahedral atom bonds, allows obtaining the largest PBG among all photonic crystals. In the Si-34 clathrate lattice, atoms are arranged in a very isotropic manner and the Brillouin zone is most close in shape to a sphere. This is favoring for the opening of the complete PBG. All of the preceding suggests that studies into the clathrate crystal lattices as candidates for photonic crystal applications show great promise. The objective of this work is to look into the possibility of creating a complete PBG in Si-34-based photonic crystals.

In our studies, we used the following model. The dielectric material is supposed to be nonabsorbing, nonmagnetic, and isotropic; i.e., the refractive index of the medium is $n=\sqrt{\varepsilon}$, where ε is the permittivity of the dielectric in the optical range. The eigenmodes of Maxwell's equations with periodic boundary conditions were computed by preconditioned conjugate-gradient minimization of the block Rayleigh quotient in a plane-wave basis, using the freely available software package MIT PHOTONIC BANDS (MPB).[25] Three cases were analyzed: (1) the lattice sites are presented by dielectric spheres in air, (2) the lattice sites are presented by hollow spheres in dielectric, and (3) neighboring lattice sites are connected with dielectric rods.

As a result of calculations, we have found that the Si-34-based photonic crystal composed of dielectric spheres in air has no large band gaps (on the order of 5% of the permittivity $\varepsilon=12$), whereas the photonic crystal composed of air spheres in the dielectric has no band gaps at all. At the same time for the lattice composed by dielectric rods and with the same value of ε the size of the PBG is about 16%. This can be pointed out as a distinguishing feature of the studied structure because usually air spheres in dielectric matrix are much more favorable for gap opening than dielectric spheres and comparable with dielectric rod structure. It can be explained as follows. In comparison with, for example, fcc or diamond grating, the studied structure has rather nonuniform distribution of atoms in spite of its high isotropy. For reasonable value of ratio between dielectric and air volumes the structure of air spheres in dielectric makes dielectric mesh disconnected. For the same reason the dielectric spheres at lattice sites also do not allow us to get connected structure. That leads to decrease in dielectric mode frequency and closes the PBG. It is well known that connectivity of two interpenetrating dielectric and air lattices is favorable for gap opening.[1] Such connectivity we get only for the case of dielectric rods connecting lattice sites. Therefore, our further research was focused on studying the photonic crystal composed of the dielectric rods in air connecting the neighboring lattice sites and thus forming tetrahedral bonds. Such a structure can be synthesized from photopolymer by two-photon absorption lithography with the length of bonds, corresponding to the PBG in the near infrared region.[8] To get sufficiently high dielectric contrast this connected polymeric lattice should be replicated by a silicon, by means of a double inversion procedure, as it was demonstrated for the case of photonic quasicrystals.[12]

Figure 2 shows the band structure of a photonic crystal at $\varepsilon=12$ and an optimal filling factor of $f=22\%$ (the ratio of the dielectric volume to the cell's total volume). Such a filling

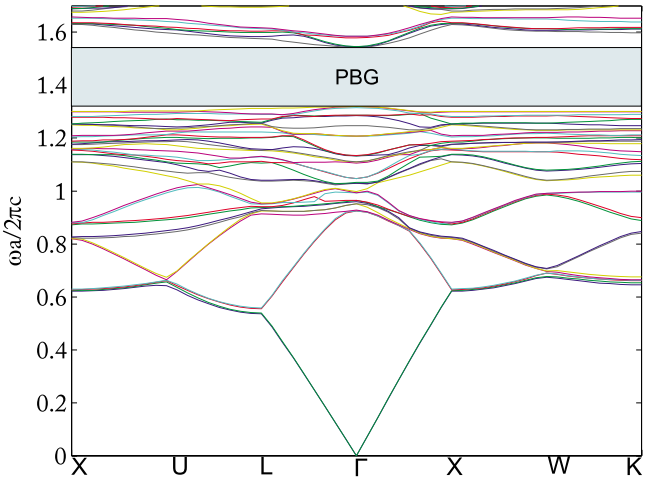

FIG. 2. (Color online) Band structure of Si-34. Permittivity: $\varepsilon=12$. Filling factor: $f=22\%$. Band-gap size: $\Delta\omega/\omega_m=15.6\%$.

factor is obtained with radius of rods equal to $r/a=0.045$, where a is the size of the cubic cell. The length of dielectric rods is equal $l/a=0.16$. The frequency is shown in the plots in the dimensionless units of $\omega a/2\pi c$, where ω is the cyclic frequency and c is the velocity of light in vacuum. On the abscissa, high-symmetry points of the fcc lattice's Brillouin zone are plotted.[26] The complete PBG is found between the 34th and 35th bands. The position of the band gap corresponds to the length of the tetrahedral atom bonds. It can be seen from comparison of the ratio of midgap frequencies of diamond and Si-34 structures and ratio of distances between the neighbor sites of these two lattices. In this sense the gap in Si-34 corresponds to fundamental gap of diamond grating. Band gap has the size of $\Delta\omega/\omega_m=15.6\%$, the filling factor being $f=22\%$. The complete PBG size $\Delta\omega/\omega_m$ is defined as

$$\Delta\omega/\omega_m = 2\frac{\min(\omega_{i+1}) - \max(\omega_i)}{\min(\omega_{i+1}) + \max(\omega_i)}100\%, \qquad (1)$$

where $\min(\omega_{i+1})$ and $\max(\omega_i)$ are the minimal and maximal frequency for the bands $(i+1)$ and (i), respectively. Thus, it is a photonic crystal with clathrate lattice symmetry with 34 atoms per unit cell that has a complete PBG.

With the aim of determining a minimal value of the permittivity ε_{th} that leads to the emergence of a complete PBG, i.e., determining the complete PBG threshold, the relation between the band-gap width and the permittivity was derived. For calculating this relation, at each permittivity value ε we derived the dielectric filling factor f corresponding to the maximal complete PBG, as shown in Fig. 3. Figure 3 shows that the complete PBG threshold is found at $\varepsilon_{\text{th}}=5.0$. This threshold value is higher than the threshold of $\varepsilon_{\text{th}}=4.0$ for a photonic crystal with diamond lattice symmetry but lower than that of the photonic crystal with the inverted opal lattice.[27] The reason is that the Si-34-based PBG structures are more isotropic so that the frequency of their boundary bands (bands bounding the PBG) weakly depends on the direction of the electromagnetic wave propagation.

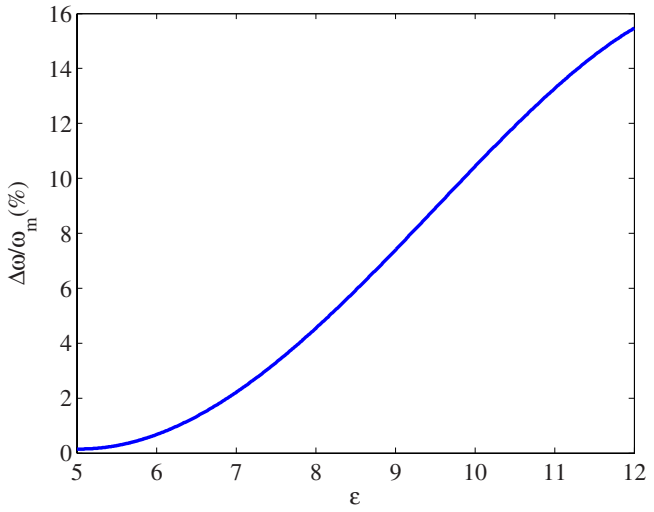

FIG. 3. (Color online) The band-gap size $\Delta\omega/\omega_m$ vs the permittivity ε.

We have studied the band-gap isotropic properties. For the photonic band (i), the isotropy parameter F was derived as follows:[28]

$$F = 2\frac{\max(\omega_i) - \min(\omega_i)}{\max(\omega_i) + \min(\omega_i)}. \quad (2)$$

Of the earlier known PhC structures, the most isotropic PBG we found was in the crystal with the fcc lattice composed of air spheres in dielectric. At $f=27\%$ and $\varepsilon=12$, such a lattice has $F=0.08$ for the "lower" band and $F=0.066$ for the "upper" band. At the same conditions $(r/a=0.051)$, a PhC with the Si-34 crystal lattice has the isotropy parameter of $F=0.022$ for the lower band and $F=0.056$ for the upper band. Thus, the PBG of the clathrate Si-34 lattice demonstrates higher isotropy. It is also found that the parameter F is monotonically decreasing with increasing permittivity.

It has been known that the group velocity of the electromagnetic waves can become zero at the PBG boundary. Physically, this means that waves scattered at the PBG boundary form a standing wave, thus making possible the emission of coherent light.[29] In the conventional PhCs this can be achieved only in certain directions, as the location of the PBG boundary is a function of the direction of the electromagnetic wave propagation. For the radiation to be coherent irrespective of the propagation direction, photonic crystals with isotropic PBG need to be used. Isotropic photonic band gaps can also be used for obtaining the omnidirectional negative refraction. This phenomenon was studied for 2D photonic crystals[30] and quasicrystals.[31]

Summing up, a complete PBG in the photonic crystal with clathrate Si-34 lattice has been revealed. The structure composed by dielectric rods has large PBG (about 16% by $\varepsilon=12$) while the PhC formed by dielectric spheres and air spheres in dielectric has small PBG (5%) and no band gap, correspondingly. The relatively low-band-gap threshold in terms of permittivity has been found to be $(\varepsilon_{th}=5.0)$. Obtained band gap is more isotropic than corresponding gap of photonic crystal with inverted opal structure.

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[1] J. D. Joannopoulos, R. D. Meade, and J. N. Winn, *Photonic Crystals: Molding the Flow of Light* (Princeton University Press, Singapore, 1999).
[2] E. Yablonovitch, Phys. Rev. Lett. **58**, 2059 (1987).
[3] J. E. G. J. Wijnhoven and W. L. Vos, Science **281**, 802 (1998).
[4] C. Cuisin, A. Chelnokov, J.-M. Lourtioz, D. Decanini, and Y. Chen, Appl. Phys. Lett. **77**, 770 (2000).
[5] M. Campbell, D. N. Sharp, M. T. Harrison, R. G. Denning, and A. J. Turberfield, Nature (London) **404**, 53 (2000).
[6] A. Blanco, E. Chomski, S. Grabtchak, M. Ibisate, S. John, S. W. Leonard, C. Lopez, F. Meseguer, H. Miguez, J. P. Mondla, G. A. Ozin, O. Toader, and H. M. Van Driel, Nature (London) **405**, 437 (2000).
[7] Yu. V. Miklyaev, D. C. Meisel, A. Blanco, G. Von Freymann, K. Bush, W. Koch, C. Enkrich, M. Deubel, and M. Wegener, Appl. Phys. Lett. **82**, 1284 (2003).
[8] M. Deubel, G. Von Freymann, M. Wegener, S. Pereira, K. Bush, and C. M. Soukoulis, Nature Mater. **3**, 444 (2004).
[9] K. M. Ho, C. T. Chan, and C. M. Soukoulis, Phys. Rev. Lett. **65**, 3152 (1990).
[10] D. N. Sharp, A. J. Turberfield, and R. G. Denning, Phys. Rev. B **68**, 205102 (2003).
[11] W. Man, M. Megens, P. J. Steinhardt, and P. M. Chaikin, Nature (London) **436**, 993 (2005).
[12] A. Ledermann, L. Cademartiri, M. Hermatschweiler, C. Toninelli, G. A. Ozin, D. S. Wiersma, M. Wegener, and G. von Freymann, Nature Mater. **5**, 942 (2006).
[13] Y. Roichman and D. G. Grier, Opt. Express **13**, 5434 (2005).
[14] W. Steurer and D. Sutter-Widmer, J. Phys. D **40**, R229 (2007).
[15] R. D. Meade, A. M. Rappe, K. D. Brommer, J. D. Joannopoulos, and O. L. Alherhand, Phys. Rev. B **48**, 8434 (1993).
[16] K. Wang, S. David, A. Chelnokov, and J. M. Lourtioz, J. Mod. Opt. **50**, 2095 (2003).
[17] P. N. Dyachenko and Y. V. Mikyaev, Proc. SPIE **6182**, 61822I (2006).
[18] M. C. Rechtsman, H. C. Jeong, P. M. Chaikin, S. Torquato, and P. J. Steinhardt, Phys. Rev. Lett. **101**, 073902 (2008).
[19] P. N. Dyachenko, Y. V. Mikyaev, and V. E. Dmitrienko, JETP Lett. **86**, 240 (2007).
[20] A. W. Rodriguez, A. P. McCauley, Y. Avniel, and S. G. Johnson, Phys. Rev. B **77**, 104201 (2008).
[21] S. David, A. Chelnokov, and J.-M. Lourtioz, Opt. Lett. **25**, 1001 (2000).
[22] T. D. M. Lee, G. J. Parker, M. E. Zoorob, S. J. Cox, and M. D. B. Charlton, Nanotechnology **16**, 2703 (2005).
[23] A. J. Garcia-Adeva, Phys. Rev. B **73**, 073107 (2006).
[24] G. B. Adams, M. O'Keeffe, A. A. Demkov, O. F. Sankey, and Y.-M. Huang, Phys. Rev. B **49**, 8048 (1994).
[25] Steven Johnson and John Joannopoulos, Opt. Express **8**, 173

(2001).
[26] A. Chutinan and S. Noda, Phys. Rev. B **57**, R2006 (1998).
[27] K. Busch and S. John, Phys. Rev. E **58**, 3896 (1998).
[28] H. Takeda, T. Takashima, and K. Yoshino, J. Phys.: Condens. Matter **16**, 6317 (2004).
[29] M. Meier, A. Mekis, A. Dodabalapur, A. Timko, R. E. Slusher, J. D. Joannopoulos, and O. Nalamasu, Appl. Phys. Lett. **74**, 7 (1999).
[30] R. Gajic, R. Meisels, F. Kuchar, and K. Hingerl, Phys. Rev. B **73**, 165310 (2006).
[31] Z. Feng, X. Zhang, Y. Wang, Z.-Y. Li, B. Cheng, and D.-Z. Zhang, Phys. Rev. Lett. **94**, 247402 (2005).