Appl. Phys. B 76, 729–734 (2003)
DOI: 10.1007/s00340-003-1169-8

Applied Physics B
Lasers and Optics

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Tetragonal photonic woodpile structures

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Received: 20 October 2002/Revised version: 31 March 2003
Published online: 24 June 2003 •

ABSTRACT The photonic properties of dielectric woodpile structures with face-centered-tetragonal (fct) and body-centered-tetragonal (bct) lattice symmetries are theoretically studied. Computational calculation of the photonic band structure reveals a photonic band gap between the second and third photonic band in both symmetries. A complete photonic band gap is not found in the bct structure due to a band gap shift with variable direction of lightflow. When the degree of layer disorder in fct woodpiles is increased, the stop bands slightly narrow and the attenuation of the optical transmission is reduced. Even so, layer-to-layer misalignment in dielectric woodpile structures may be tolerable up to 20%–30% in most applications. The complete photonic band gap in fct woodpiles remains open with planar layer-to-layer disorder up to 60%–70%.

PACS 42.70.Qs; 78.20.Bh; 78.20.Ci

1 Introduction

Woodpile or logpile structures are three-dimensional photonic crystals (PCs) built by blocks or rods that are orthogonally stacked together. The blocks are embedded in a medium with a higher or lower dielectric constant. The shape of the blocks can be spherical, cuboidal, or ellipsoidal. The blocks may touch each other, may overlap or be detached to a certain extent. The photonic properties of woodpile structures are affected by the refractive index contrast between the material of the blocks and the embedded medium, as well as by the structural geometry of the photonic unit cell. Typically, the blocks in the woodpile structure are square-shaped in cross-section and made of a material with a high dielectricity embedded in air.

The woodpile structure with a face-centered-tetragonal (fct) lattice symmetry was first presented by Ho et al. and further realized by several other groups [1–7]. The unit cell contains a stack of four layers, in which the third and fourth layers are shifted by half of the periodicity compared with the first and second layers, respectively. The blocks are aligned along the [110] and [$1\bar{1}0$] directions, with [001] as the stacking direction. The unit cell is cubic with an aspect ratio of $\sqrt{2}$, the ratio between the unit cell height and the pitch of the line pattern. With higher or lower aspect ratios the unit cell carries the tetragonal lattice symmetry. The fct woodpile structure has a complete photonic band gap along all directions of light propagation. The midgap frequency of the stop band is scalable by the lattice parameter of the photonic crystal. By varying the filling fraction, which is the ratio of the width of the square-shaped rods to the pitch, the size of the complete photonic band gap can be maximized. The aspect ratio of the structure is a valid tuning parameter for energetically adjusting local gaps.

Omnidirectional photonic band gaps, which cover the conventional C-band for international telecommunication ranging from 1.53 to 1.57 μm, are of great interest and require fabrication of the photonic crystal in the sub-micron range. For a complete band gap at 1.55 μm, the rod dimensions of the fct woodpile structure are of $0.16 \times 0.19\,\mu m^2$ with a pitch of 0.62 μm between adjacent rods [8].

If the third and fourth layers of the woodpile's unit cell are aligned identically to the first two layers without a shift in the plane, another type of woodpile structure is developed. This woodpile has body-centered-tetragonal (bct) crystal symmetry. The bct woodpile structure can be transformed into the fct structure by a shift of the blocks in the third and fourth planes normal to the stacking direction. Therefore, the bct woodpile structure can be interpreted as an fct woodpile with the highest degree of layer-to-layer disorder.

The bct and fct woodpile structures are shown schematically in Fig. 1. For both woodpile structures, a stop band in the transmission spectrum was experimentally found in the GHz range by Özbay et al. using robust metallic rods [9]. They found an average attenuation of the transmission of 7–8 dB per layer for both structures along the stacking direction.

In the layer-stacking fabrication of woodpile structures, either by the deposition method of Lin et al. [6] or by the wafer-bonding approach of Noda et al. [8], fabrication-related defects are difficult to avoid. In particular, the exact alignment of the line-pattern in woodpile structures over large areas is critical. For sub-micron fabrication with exact planar alignment of the layers, diffraction observation methods

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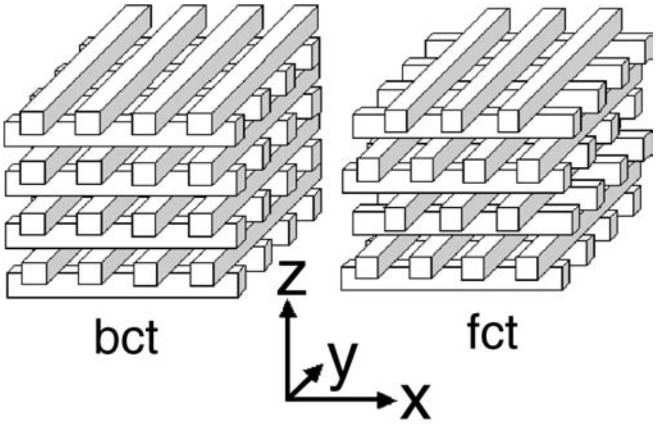

FIGURE 1 Schematic drawing of woodpile structures with body-centered-tetragonal (bct, *left*) and face-centered-tetragonal (fct, *right*) lattice symmetries. The woodpile stacking direction is parallel to the z-axis

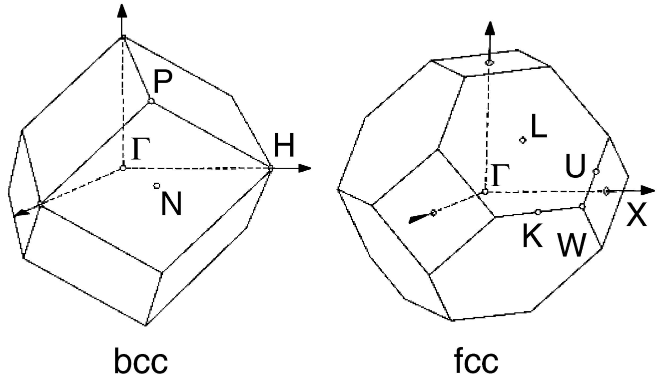

FIGURE 2 The corresponding reducible Brillouin zone of the bcc (*left*) and fcc (*right*) photonic woodpile structures with their associated symmetry points

are used [10]. This requires the implementation of alignment marks and an instrumental setup for the optical observation and precise movable specimen holders. While attenuation of the transmission has been found in fct as well as in bct woodpile structures, stop bands may be found for all interstructural symmetries. Consequently, if complete photonic band gaps are found in all woodpile structures, fabrication of applicable three-dimensional PCs might be possible without precise alignment techniques. This would reduce costs and time in industrial three-dimensional PC fabrication.

2 Geometry and symmetry considerations

The woodpile structure with bct lattice symmetry corresponds to a fct arrangement with the highest degree of layer-to-layer disorder in the third and fourth planes of the unit cell. The shift parameters δ_x and δ_y characterize the plane shift of the layers along the [110] and [1$\bar{1}$0] directions, the denoted x- and y-directions, respectively. With $\delta_x = 0.5a$ and $\delta_y = 0.5a$ the structure yields the perfect fct woodpile structure, where a is the pitch between the stripes of the line-pattern or the periodicity of the dielectric structure. By varying the shift parameters δ_x and δ_y, all interstructural geometric arrangements of woodpile structures between the fct and bct are feasible.

The fct woodpile structure has a face-centered-cubic (fcc) primitive unit cell if the aspect ratio $c/a = \sqrt{2}$, where c is the height of the unit cell and a is the translational periodicity perpendicular to the stacking direction. Since the unit cell contains four layers, the height of each layer is $c/4$. The photonic structure can be derived from the zinc-blende crystal lattice by replacing the sulfur-center of the tetraeder sites at (3/4, 1/4, 1/4), (1/4, 3/4, 1/4), (1/4, 1/4, 3/4), and (3/4, 3/4, 3/4) by the [1$\bar{1}$0] line-pattern and replacing the zinc-edges of the tetraeder sites by the [110] crossed line-pattern. Analogous considerations yield the woodpile structure with body-centered-cubic (bcc) lattice symmetry. By replacing the {1, 0, 0} edges of the unit cell by the [1$\bar{1}$0] line-pattern and the {1/2, 1/2, 1/2} positions by the crossed [110] line-pattern, the associated bcc woodpile structure is developed. The bcc unit cell contains two layers with the aspect ratio of $\sqrt{2}$. The direction parallel to the [110] line pattern is represented by the x-axis, whereas the y-axis is directed along the [1$\bar{1}$0] line pattern. The stacking direction is denoted as the z-axis [001]. The unit cell of the fcc structure is twice as large as that of the bcc structure along the stacking direction for the same periodicity a. Away from the aspect ratio of $\sqrt{2}$, the cubic structures have tetragonal lattice symmetries.

In analogy to scattering of electrons by a periodic atomic potential in solid state physics, the cross-section of photon scattering is reflected by the symmetry of the photonic structure. The final states of photons scattered in dielectric periodic structures considering crystallographic symmetry relations are catalogued by the photonic band structure (PBS). For all wavevectors of the incident electromagnetic waves the PBS yields the allowed photonic states of the dielectric structure. The bands in the PBS are considered along the edges of the irreducible Brillouin zone (BZ). Points, which belong to irreducible groups of high symmetry, are denoted with Latin and Greek characters. The irreducible symmetry representations of the fcc crystal structure are given by the symmetry points X, U, L, Γ, W, and K, which belong to the symmetry groups D_{4h}, C_{2v}, D_{3d}, T_d, D_{2d}, and C_{2v}, respectively, using the Schönflies notation. The irreducible BZ of the fcc lattice is a polyhedron, the edges of which are the symmetry points given above. Symmetry points of the irreducible BZ, which carry the bcc crystal structure, are given by Γ, N, H, and P or T_d, D_{2h}, O_h and T_d, respectively. The reducible BZs corresponding to the fcc and bcc crystal lattices are shown in Fig. 2. In the tetragonal arrangements additional symmetry points must be considered along the direction of the tetragonal distortion.

3 Calculation of the photonic properties

Optical transmission spectra of woodpile structures were calculated using a modified computer code of the transfer matrix method by Bell et al. [11]. The code was modified to woodpile structures with layer-to-layer disorder in the x- and y-direction. The considered unit cell was projected onto a three-dimensional grid with up to 1400 mesh points for sufficient computing convergence. The calculated spectra were accomplished using dielectric layers of square-shaped rods with a refractive index of 3.4, the refractive index of silicon at 1.5 μ m at the wavelength for optical telecommunication. For calculation of the transmission spectra the lightflow was directed along the x-, y-, and z-direction, respectively. The z-direction is the stacking direction denoted by $\Gamma X'$ in the fct and by $\Gamma H'$ in the bct structure, analogous to ΓX and ΓH in the cubic arrangement. Due to the lattice symmetry of the fct and bct structures, the physical properties along the x- and the y- direction cannot be distinguished. Thus, the degenerate x- and y- directions, which are the [011] and [0$\bar{1}$1] directions in real space, are considered as the ΓK direction in the fct and as the ΓN direction in the bct reducible BZ.

While changing the degree of disorder by shifting the third and fourth layers of the woodpile's unit cell in the x–y plane, optical transmission spectra of the fct structure were calculated along ΓK and $\Gamma X'$. The aspect ratios c/a were varied in the range 0.8 to 1.4 with a filling fraction ranging from 20 to 40%. Attenuation of the transmission was found in all spectra regardless of the disorder of the dielectric structure. With increasing degree of disorder the stop band of the not-disturbed fct arrangement closes, while at lower frequencies a second stop band opens. In the highly disordered fct woodpile along ΓK, which is the ΓN direction in the bct arrangement, only the second band remains. In between the well-ordered and highly disordered arrangement two photonic stop bands, with an energetic midgap distance of 0.13 in normalized frequencies, exist simultaneously. The distance between the midgap frequencies remains unchanged for all considered aspect ratios and independent from the filling fraction.

Along the stacking direction $\Gamma X'$ the position of the midgap frequency remains constant with increasing misalignment of the third and fourth layers in the x–y plane of the photonic unit cell. The size of the stop band slightly decreases from the fct to the bct arrangement. Representative transmission spectra are summarized in Fig. 3. The polarization of the incident electromagnetic field along the stacking direction, either of the TE or the TM mode, are rejected separately, depending on their associated shift parameter, δ_x or δ_y. Perpendicular to the stacking direction the TE and TM mode are coupled to both shift parameters.

Increasing the number of layers leads to a significant rise of the attenuation during lightflow propagation in woodpile structures. The midgap attenuation of the calculated transmission in woodpile structures was considered as a function of the number of periods or unit cells. The aspect ratio c/a was varied from 0.8 to 1.4 with filling fraction ranging from 20 to 40%. In the undisturbed fct woodpile structure a maximal attenuation per period of 10–13 dB was observed for both transversal modes along the $\Gamma X'$ direction. Along ΓK a maximal attenuation of 4 and 7 dB per period was found for the TE mode and TM mode, respectively. In woodpiles with bct lattice symmetry, a 3 dB attenuation per period was achieved for both transversal modes along ΓN. Along the stacking direction $\Gamma H'$, attenuation of the transmission for both modes decreased with decreasing aspect ratios 1.4, 1.2, 1.0, and 0.8 from 5 to 3 dB per unit period. The results for the bct woodpile arrangement are summarized in Fig. 4. While varying the filling fraction, the gap to midgap ratios were considered for lightflow along $\Gamma X'$ and ΓK in the fct and along $\Gamma H'$ and ΓN in the bct woodpile structures with an index of refraction contrast of 3.4 : 1. The gap to midgap ratio $\Delta w/w_g$ determines the ratio of the width of the stop band to the center of the gap. The maximum of the local gap to midgap ratio in bct woodpiles of $\Delta w/w_g = 31\%$ was observed with a 26% filling fraction along the stacking direction $\Gamma H'$. Along ΓN, a maximum gap to midgap ratio of $\Delta w/w_g = 43\%$ was observed for a 33% filling fraction. This result remains valid for aspect ratios c/a

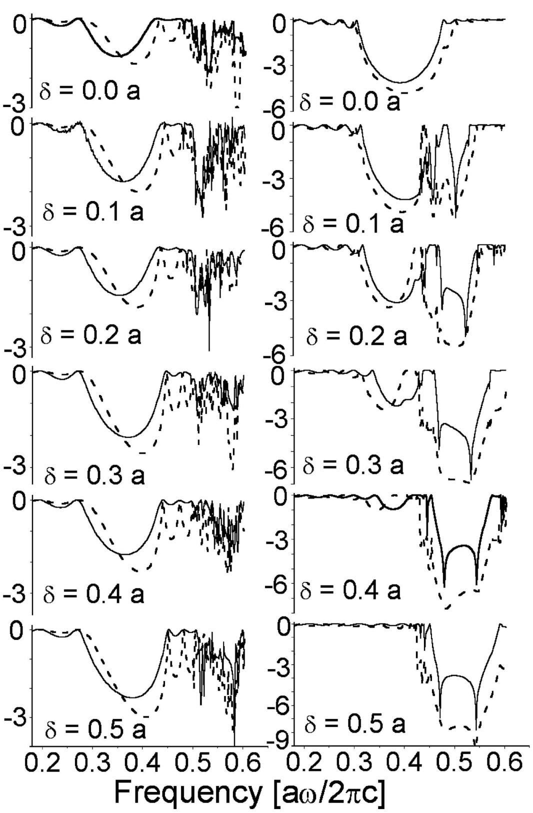

FIGURE 3 Calculated optical transmission spectra of the TE (*solid line*) and TM (*dashed line*) of the fct photonic woodpile structure with increasing misalignment of the third and fourth layers. The shift parameter δ ($\equiv \delta_x = \delta_y$) is given in units of the photonic crystal periodicity a. The lightflow was directed along the stacking direction (*left*) and perpendicular to the stacking direction (*right*). The attenuation unit is given in dB. The aspect ratio of the photonic unit cell was 1.2

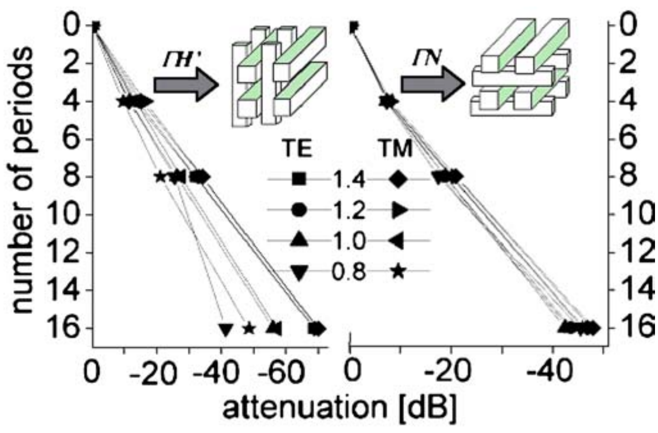

FIGURE 4 Calculated attenuation per period in dielectric woodpile structures with bct lattice symmetry for aspect ratios ranging from 0.8 to 1.4. The lightflow transmission was considered along (*left*) and perpendicular (*right*) to the stacking direction

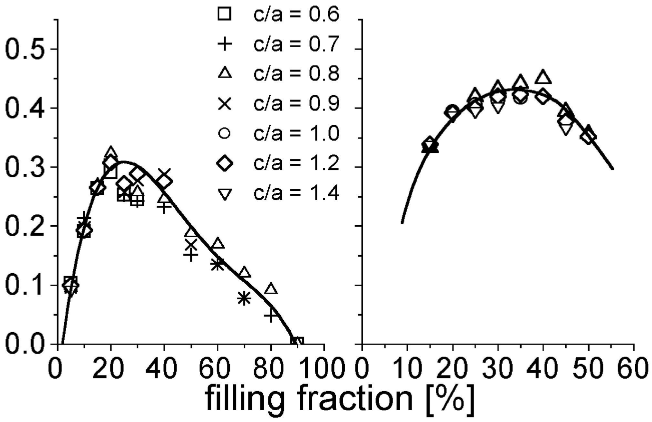

FIGURE 5 Local gap to midgap ratios with varying filling fractions and various aspect ratios c/a for transmission along (*left*) and perpendicular (*right*) to the stacking direction. The calculations were performed by means of a dielectric woodpile structure with bct lattice symmetry

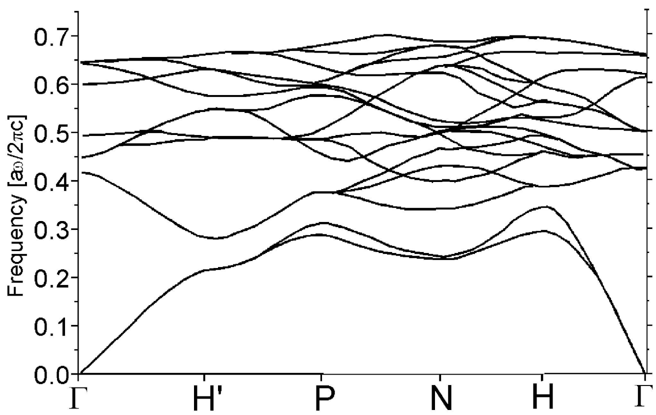

FIGURE 6 Calculated photonic band structure of the dielectric woodpile structure with body-centered-tetragonal lattice symmetry. Between the second and the third band, a photonic band gap is found for all directions, but the band gap is not complete

ranging from 0.6 to 1.4. Beyond this valid range, the gap to midgap ratio decreases significantly. The bct gap to midgap ratio versus the filling fraction is given in Fig. 5 for lightflow directions along $\Gamma H'$ and ΓN.

In addition to optical transmission spectra, the photonic band structure (PBS) carries important information on the photonic properties of periodic dielectric structures. While the calculated transmission spectra can be directly compared with the experiment, the PBS is a theoretical model to yield the photonic states within the infinite periodic dielectric structure. The PBS of the woodpile structure with fct lattice symmetry has already been calculated in numerous articles (See for example, [2, 3, 12–15]). The PBS of the bct woodpile structure has not been presented so far. In Fig. 6 the calculated PBS for the bct arrangement is shown, assuming a periodic structure with a refractive index contrast of 3.4 : 1, a filling fraction of 23%, and a bct unit cell with a height-to-pitch ratio of 1.2.

4 Discussion of the results

From the photonic band structure (PBS) calculations, a photonic band gap is observed in the bct woodpile structure between the second and third photonic bands for all directions. The photonic band gap, however, is not complete. By decreasing the aspect ratio of the bct unit cell, the local gap between the second and the third photonic band at the symmetry point H' can be shifted to match energetically with the symmetry point H. While changing the aspect ratio, the band gap along the symmetry points PN closes. The appearance of an incomplete photonic band gap is due to the change of the bct structural periodicity along different crystallographic directions. Changing the wavevector of the lightflow from N to H and from H' to P the periodicity is increased by a factor of $\sqrt{2}$, and the midgap frequencies of the photonic gaps do not overlap. The cross-section normal to the $\langle 110\rangle$ directions (the ΓN direction) of the three-dimensional dielectric structures with bct lattice symmetry yields a square lattice in two dimensions. In structures with fct lattice symmetry the cross-section reveals a triangular 2D lattice. Similar results are observed if the cross-section normal to the $\langle 100\rangle$ directions of the bct (ΓH) and fct (ΓX) dielectric structures is considered. In analogy to the 2D photonic crystal with a square lattice, which does not have a complete band gap, the associated bct woodpile structure has no complete photonic band gap either. The triangular 2D arrangement, however, exhibits a complete gap in agreement with the dielectric woodpile, which carries the fct lattice symmetry [16, 17]. Small layer-to-layer misalignment and misalignment of the intersectional angle between the crossed layers within 10 degrees slightly change the optical and photonic properties in woodpile structures [18–20]. On the other hand, geometrical fluctuations from the desired structure and surface roughness can close the photonic band gap in inverse opals [21]. By shifting the third and fourth layers of the fct woodpile unit cell in the x–y plane, the stop band of the transmission spectrum slightly narrows and the attenuation decreases for propagation along $\Gamma X'$. The effect of misalignment along a single direction, either the x- or y-directions, is strongly coupled to the direction of the electric field of the lightflow. If the lightflow propagates along the ΓK direction, the stop band splits into two separate bands. While the stop band associated with the well-ordered fct structure closes during transformation from the fct to bct woodpile structure, a second band associated with the well-ordered bct structure opens. For the interstructural symmetries, two stop bands exist simultaneously. Along the stacking direction $\Gamma X'$, however, a shift of the midgap frequency was not observed between the fct and bct lattice symmetries, regardless of arbitrary aspect ratios and filling fractions. The complete photonic band gap in disordered fct woodpiles structures remains existent until 60%–70% degree of disorder .

Based on the calculations, the photonic properties in layer-to-layer disordered structures with 20%–30% disorder are not significantly affected. Therefore, precise layer adjustment by complex alignment facilities is not required for many applications in woodpile-based photonics. The reduction of the gap size associated with the increasing disorder may be tolerable, in particular, if the application considers only light propagation parallel to the stacking direction. A complete photonic band gap, however, is not found in highly disordered structures with bct lattice symmetry.

In fct and bct woodpile structures the attenuation of the optical transmission increases with the number of layers. The average attenuation per unit cell in fct woodpiles structures along the stacking direction $\Gamma X'$ has been reported by different groups. Experimentally, Lin et al. revealed an average attenuation per unit cell of about 12 dB for comparable structural geometries and index contrast [6]. Noda et al. achieved up to a 23 dB maximal attenuation per unit cell in their fct woodpile structure made of GaAs [5]. Özbay et al. observed a 17 dB attenuation per unit cell in metallic woodpiles working in the GHz range [4]. Ho et al. experimentally measured a 17 dB and theoretically obtained a 21 dB attenuation per unit cell [1]. Whittaker calculated an attenuation of approximately 12 dB per unit cell along the stacking direction $\Gamma X'$ [12]. Similar results were observed in the present calculations based on woodpiles with the bct and fct lattice symmetries. The results may vary due to the different aspect ratios of the unit cell and refractive index contrast. Along the $\Gamma X'$ direction in fct woodpiles an average attenuation per unit cell of 10 dB was observed for both transversal modes with aspect ratios ranging from 0.8 to 1.0. Up to 13 dB was observed for aspect ratios around 1.2 to 1.4. Perpendicular to the stacking direction along ΓK, an average attenuation of 4 dB per unit cell was observed for the TE mode and 7 dB per unit cell for the TM mode. The average attenuation in woodpiles with bct lattice symmetry is significantly reduced compared with fct woodpiles. A maximum attenuation per unit cell of about 5 dB was found for the TE and the TM mode along the stacking direction $\Gamma H'$. Perpendicular to the stacking direction, along ΓN, an attenuation per unit cell of less than 3 dB was found for both transversal modes and various aspect ratios.

Since a considerable attenuation of the transmission is observed in fct woodpiles along the stacking direction within only a few periods, many more periods are required to observe comparable attenuation in woodpiles with bct lattice symmetry. Perpendicular to the stacking direction, where the number of periods is generally large, the maximal attenuations of the transmitted light in fct and bct woodpiles are equivalent. Practically, in sub-micron fabrication of woodpile structures, in which the structures are either realized by the wafer-bonding technique or by layer deposition, the adding of stacking periods is the challenge for obtaining a desired attenuation of more than 50 dB.

The maximal gap to midgap ratio $\Delta w/w_g$ in woodpiles with bct lattice symmetry obtained from the calculations are close to the reported gap to midgap ratios for fct woodpiles along the stacking direction. In this study the maximal gap to midgap ratio for bct woodpiles was 0.31 at a 25% filling fraction along $\Gamma H'$. Gap to midgap ratios for fct woodpiles along the stacking direction have been reported to be 0.36–0.40 for 26%–29% filling fractions with a refractive index contrast ranging from 2.8 : 1 to 3.6 : 1 [1, 4, 6, 7, 22]. Along ΓN, a maximum gap to midgap ratio of $\Delta w/w_g = 43\%$ was observed with a 33% filling fraction in the bct woodpile structure.

The results based on the described theoretical layer-by-layer stacking approach may weaken the tight framework for the design of three-dimensional photonic crystals of actual technological interest at sub-micron dimensions. The small effect on the optical properties of slightly misaligned dielectric fct structures with complete photonic band gaps allows industrial fabrication of applicable optical devices without handling the problem of structural imprecision by sophisticated alignment instrumentation. A measurable influence on the optical and photonic properties of dielectric fct woodpiles due to layer misalignment should not matter below a 20%–30% planar shift from the theoretical prediction. While woodpiles with fct lattice symmetry are purely artificial, the bct woodpiles are naturally existent as zeolites. Although, the periodicity of zeolite structures of about 50–100 nm is too small for applied photonics in the frequency range of current technological interest, they are probably suitable as templates for three-dimensional photonic crystal systems.

5 Summary and conclusion

The photonic properties of three-dimensional woodpile structures were theoretically studied in terms of layer-to-layer disorder, varying aspect ratios, filling fractions, and number of periods. The body-centered-tetragonal (bct) woodpile structure is derived from the face-centered-tetragonal (fct) lattice symmetry by shifting the layers of the third and fourth planes of the photonic unit cell. The bct woodpile structure can be understood as a fct woodpile with highest layer-to-layer misalignment. Like the dielectric structure with fct lattice symmetry, the bct structure exhibits a photonic band gap between the second and third photonic bands. The gap, however, is not complete. Transfer from the fct to the bct woodpile structure leads to a shift of the midgap frequency to lower frequencies perpendicular to the stacking direction. The average attenuation of the transmission of the lightflow along this direction remains unchanged. Along the stacking direction, however, the attenuation in bct woodpiles per unit cell is decreased by several orders of magnitude. Results are given for various aspect ratios and filling fractions of the photonic unit cell. In bct woodpiles the size of the photonic stop bands is slightly smaller than the associated stop bands for the fct geometry. To compensate for the effect of layer-to-layer disorder, more stacking layers are necessary along the stacking direction.

In conclusion, layer-to-layer misalignment in dielectric woodpile structures may be tolerable to a considerable extent. The complete photonic band gap associated with the fct woodpile structure closes not before 60%–70% layer-to-layer misalignment. For most applications, disorder up to 20%–30% may be acceptable. If the applied lightflow of interest is directed parallel to the stacking direction, the impact of layer-to-layer disorder on the photonic properties of woodpile structures is limited to the decrease of the attenuation of the optical transmission.

ACKNOWLEDGEMENTS This work is part of the German Research Foundation (DFG) Project No. ZA191/13-1. R. Hillebrand and M. Zacharias are acknowledged for helpful discussions.

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