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Absolute three-dimensional photonic band gap in the infrared regime in woven structures

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We closely study the formation of a three-dimensional (3D) photonic band gap in a system composed of dielectric fibers. The fibers are woven into layers that are then stacked up to form 3D lattices of different structures. The woven systems have the advantage of easy fabrication and, with the cross sections of fibers in microns, the band gap can be made in the infrared regime. We employ the transfer-matrix method to study the photonic band structures. The optimized gap-formation condition is found in a quasi-body-centered-cubic structure. A 3D full gap is identified in the middle infared regime with the use of fibers of moderate dielectric constants ($\epsilon \leqslant 16$). Our studies strongly suggest the possibility of employing such woven structures in various photonic insulator-related applications. [S0163-1829(99)50216-6]

In 1989 Yablonovitch and Gmitter first demonstrated that, analogous to electrons in crystals, electromagnetic (EM) waves exhibit band structures in periodic dielectric materials.[1] In a photonic band gap (PBG), EM waves scattered by the periodic dielectric decay exponentially[2] and therefore, propagations are forbidden. This phenomenon not only leads to new interests in quantum electrodynamics, but also arouses intensive studies on its potential applications,[3] such as in controlling spontaneous emission.[4,5] However, due to the vector nature of the EM waves, bands of different polarizations are generally nondegenerate and thus have gaps at different energies, which makes an absolute band gap difficult to form. Many artificial PBG systems have been studied,[3] but they mostly produce gaps only in limited directions. Finding a realistic photonic structures with an absolute three-dimensional (3D) gap is highly desirable.

The PBG systems were first studied in the microwave regime and were later extended to the infrared. A PBG in the infrared or even the visible regimes could facilitate many practical laser applications and is, thus, technologically important as well as scientifically interesting. This, however, requires the lattice size to be reduced to microns, which is difficult to achieve with the currently available drilling or etching methods.[3,6] Other fabrication techniques were proposed, such as the layer-by-layer method,[7] holographic technique,[8] or other combinations.[9] Recently, a 3D absolute gap in the far infrared has been identified,[10] but so far only 2D photonic gaps have been obtained in the visible regime.[8,11] Forming 3D absolute photonic gaps in higher frequency ranges remains a task to be realized.

In this paper, we propose a 3D woven structure for such a goal. The system is composed of dielectric fibers woven into identical patterns and then stacked up into a 3D lattice. Fibers with cross sections in micrometers have been available for years (e.g., optical fibers[12]) and weaving is a simple technology known for centuries. Weaving such fibers into fabric for designed optical properties seems both promising and feasible. Meanwhile, with the use of fibers, woven technique may provide an alternative way to build the layer-by-layer structures in micrometers that are currently fabricated by the more complicated etching process.[10] Our previous study[13] has shown that fibers woven into a rectangular lattice can indeed produce a full 3D photonic band gap in the middle infrared regime. This structure, however, requires fibers of large dielectric constant ($\epsilon \geqslant 40$) which, although available,[12] restricts its possible applications.

In this paper, we report the formation of an absolute band gap in a woven system that only requires modest dielectric constants ($\epsilon \sim 16$). To achieve this, we design a structure with a larger packing fraction and more spherical Brillouin zones than the earlier one.[13] We also employ two different fibers to take advantage of its better symmetry properties. The vector-wave transfer-matrix method[14] is applied to calculate the band structures and the constant-frequency dispersion surface scheme[15] is employed to examine the completeness of the gap opening. The results confirm a 3D full photonic gap in the middle infrared range for this woven structure of moderate dielectric constants. The optimal structure for this system to become a photonic insulator is also studied.

The woven structure is composed of two fibers of dielectric constant ϵ_1 and ϵ_2. They have the same diameter d, and are woven into a hashlike pattern shown in Fig. 1(a), which is the building block for the photonic crystal. The whole fabric is embedded in a background medium of dielectric constant ϵ_b (here taken to be vacuum). The center of the fibers in such a unit can be described by

$$\left[x, \frac{A}{4}, h \sin\left(\frac{2\pi}{A}x\right)\right] \text{ and } \left[-\frac{A}{4}, y, h \sin\left(\frac{2\pi}{A}y\right)\right] \text{ for } \epsilon_1 \tag{1}$$

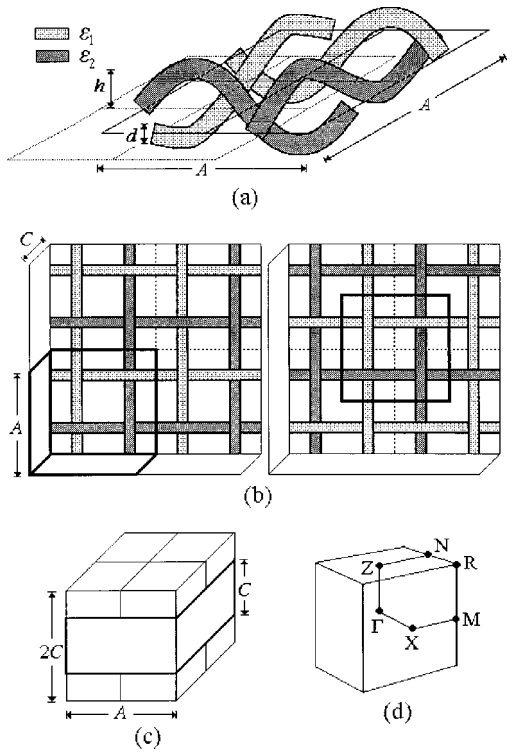

FIG. 1. (a) Building block of a woven structure. (b) Down view of two adjacent woven layers in which the building block is denoted by boldfaced areas. Curvatures of the fibers are ignored for the convenience of plotting. (c) Unit cell, and (d) first Brillouin zone of the rectangular woven structure.

and

$$\left[x,-\frac{A}{4},-h\sin\left(\frac{2\pi}{A}x\right)\right] \text{ and } \left[\frac{A}{4},y,-h\sin\left(\frac{2\pi}{A}y\right)\right] \quad \text{for } \epsilon_2 \quad (2)$$

where A is the lattice constant in both the x and y directions, and h is the variation amplitude of the fiber in the z direction. Let C denote the thickness of each block in the z direction. The relations $h \geqslant d/2$ and $2h+d \leqslant C$ must be satisfied. Note that C need not equal A, i.e., the block is in general rectangular. The block repeats itself two dimensionally to form a fabric layer, which is then stacked up one above another for a 3D lattice structure. If we stack the woven layers with perfect alignment, we obtain a simple rectangular lattice with each block as the unit cell of the lattice.[13] In this paper, however, to make the Brillouin zone more spherical, we shift the second layer by $A/2$ in both the x and y directions as illustrated in Fig. 1(b). This structure is a centered-tetragonal lattice whose unit cell is twice the size of the block [Fig. 1(c)]. Two different dielectrics are needed to construct the desired centered-tetragonal lattice, since, otherwise, the shifting of the second layer would not change the crystal structure. The use of two different dielectrics reduces the C_4 symmetry about the z axis and hence removes the symmetry-induced degeneracy problem in our previous study.[13] This proves to be essential for the formation of an absolute gap (see later).

Let $\lambda = 2C/A$ denote the ratio between the height and the width of the rectangular unit cell. λ can be varied for different lattice structures. With $\lambda = 1$, we have a body-centered-cubic (bcc) lattice with a lattice constant A. Similarly, if $\lambda = \sqrt{2}$, the system can be regarded as a face-centered-cubic (fcc) lattice with a lattice constant $\sqrt{2}A$. The band structures of both systems have been studied and we find the bcc structure a better candidate as far as the band-gap formation is considered.

The band structure of these systems are calculated by the vector-wave transfer-matrix method[14] that has been successfully applied to many periodic dielectric systems.[13,15] To obtain an absolute gap, we first need a structure whose frequencies at various Brillouin-zone boundaries are close to each other, so that local gaps there can be easily aligned. Woven structures have the advantage that gap positions can be easily adjusted by varying λ. Figure 2(a) depicts the band structure of a rectangular lattice with $\lambda = 10/7$ and a uniform dielectric constant. The arrows therein indicate the high-symmetry points where we wish to align the gaps. In Table I, we summarize the centers of the most relevant high-symmetry points for different λ's. $\mathbf{X}^*$ is a k point between $\mathbf{\Gamma}$ and $\mathbf{X}$, where the bands cross and need to open up for an absolute gap. This table clearly suggests that fcc structure ($\lambda = \sqrt{2} \simeq 10/7$) would be the favorable choice since its Brillouin zone is closest to a sphere.[6] However, it turns out to be not so as will become clear later.

Figures 2(b) and 2(c) illustrate the calculated band structures for bcc and fcc, respectively. Here we have tested and employed the optimal structure parameters in favor of an absolute gap while keeping the dielectric constants in moderate range ($\epsilon_1 = 16.0$, $\epsilon_2 = 2.5$). Here and later, the dispersion surface scheme[13,15] is employed together with the transfer-matrix calculation to monitor the development of 3D band gaps. The calculation shows a full gap of size about 6% of the gap center frequency is formed in the bcc structure, but none is found in the fcc case with moderate dielectric constants. This surprising result is related to the fact that the woven structure is layered and hence highly anisotropic. Its dielectric modulation differs at various directions and therefore it is difficult to have a gap wide enough to overlap others at certain symmetry points. Meanwhile, since EM waves are vector fields, both polarizations have to be considered for the completeness of solutions. In an isotropic dielectric medium, waves of different polarizations are generally nondegenerate (see later). The band curves of the woven system would split furthermore due to this polarization-dependent effect.

Considering the effect of a single Bloch scattering potential, $U_{\mathbf{G}}$, is useful in addressing the issues here. For scalar waves like electrons in a solid, $U_{\mathbf{G}}$ would open a gap at $\mathbf{k} = \mathbf{G}/2$, but would usually have minimal effects on waves with $\mathbf{k}' \perp \mathbf{G}$. The propagation of an EM field is more complicated. The effect $U_{\mathbf{G}}$ has on the ($\mathbf{k}' \perp \mathbf{G}$) waves is polarization dependent and could be strong.

Let us put $\epsilon(\mathbf{r}) = \bar{\epsilon} + \epsilon' \cos(Gz)$ and consider an EM wave propagating in the $\mathbf{k} \| \hat{\mathbf{x}}$ direction. The TE mode waves, which are polarized in the y direction and thus $\nabla \cdot \mathbf{E} = 0$, can be described by the equation

$$\mathbf{E}(\mathbf{r}) = \hat{\mathbf{y}}\{E_k e^{ikx} + E_{k\pm G} e^{i(kx \pm Gz)}\}, \quad (3)$$

and the dispersion relation is approximately given by[16]

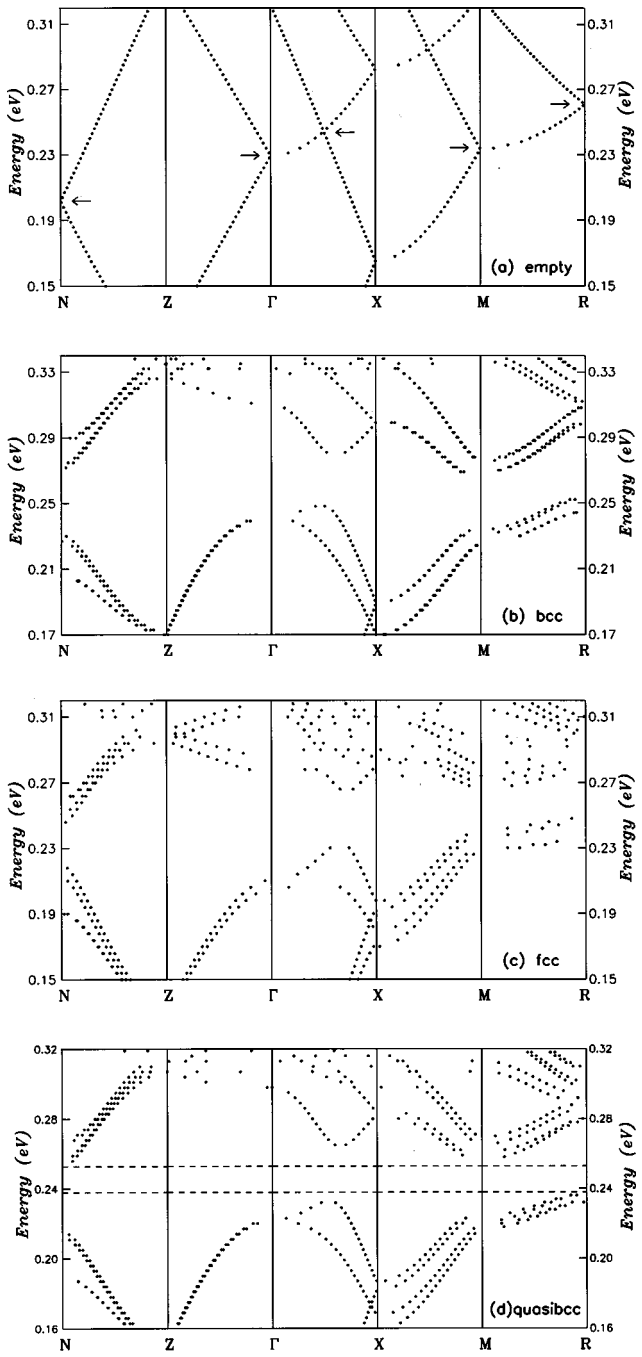

FIG. 2. Calculated photonic band structures for (a) an empty fcc lattice; (b) a bcc lattice where $h=0.12A$, $d=0.24A$, $\epsilon_1=16.0$, and $\epsilon_2=2.5$; (c) a fcc lattice where $h=0.18A$, $d=0.22A$, $\epsilon_1=20.0$, and $\epsilon_2=4.0$; (d) a quasi-bcc woven lattice where $\lambda=10/9$, $h=0.13A$, $d=0.26A$, $\epsilon_1=16.0$, and $\epsilon_2=2.5$. In all cases, $A=1.87$ μm. A full gap of a size about 7% of the gap center is found in the quasi-bcc lattice.

$$\det\begin{pmatrix} k^2-\frac{\omega^2}{c^2}\overline{\epsilon} & -\frac{\epsilon'}{2}\frac{\omega^2}{c^2} \\ -\frac{\epsilon'}{2}\frac{\omega^2}{c^2} & k^2+G^2-\frac{\omega^2}{c^2}\overline{\epsilon} \end{pmatrix}=0. \tag{4}$$

Equation (3) does not hold for the TM modes that have the **H** field polarized in the y direction and thus $\nabla\cdot\mathbf{E}\neq 0$. Instead, it would be more convenient to work with the **H** field[17]

$$\mathbf{H}(\mathbf{r})=\hat{\mathbf{y}}\{H_k e^{ikx}+H_{k\pm G}e^{i(kx\pm Gz)}\} \tag{5}$$

which, to the same order of approximation as used in deriving Eq. (4), would yield a very different dispersion for the TM mode:[16]

$$\det\begin{pmatrix} k^2-\frac{\omega^2}{c^2}/c_0 & \alpha k^2 \\ \alpha k^2 & k^2+G^2-\frac{\omega^2}{c^2}/c_0 \end{pmatrix}=0, \tag{6}$$

where

$$\alpha=-\frac{\overline{\epsilon}}{\epsilon'}+\sqrt{\left(\frac{\overline{\epsilon}}{\epsilon'}\right)^2-1}, \quad \text{and} \quad c_0=\frac{1}{\sqrt{\overline{\epsilon}^2-\epsilon'^2}}. \tag{7}$$

In other words, the TE and TM modes have their respective E fields experiencing different environments, which lead to very different band dispersions. Equations (4) and (6) are exact in their respective small k limits and we can estimate the velocities for both polarizations:

$$v_{\mathrm{TE}}=\frac{c}{\sqrt{\overline{\epsilon}}} \quad \text{and} \quad v_{\mathrm{TM}}=\frac{c}{\sqrt{\overline{\epsilon}}}\left[1-\left(\frac{\epsilon'}{\overline{\epsilon}}\right)^2\right]^{-1/4}, \tag{8}$$

i.e., waves of the TM mode travel faster than those of the TE mode. This result essentially explains the band splitting, say in Fig. 2(b), between the **Γ** and **X** points, with the smaller (larger) sloped branches for the TE (TM) mode.

This single scattering potential approximation provides a simplified picture for the complicated 3D woven structure since it is layered and, hence has a dominating $U_{\mathbf{G}_1}$ with $\mathbf{G}_1=2\pi/C\hat{\mathbf{z}}$. In our study, $U_{\mathbf{G}_1}$ is 25% larger than other Fourier components. That the bands between **Z** and **Γ** are nearly degenerate could be understood on the same grounds. The system is symmetric, apart from a phase difference, between the x and y directions. The EM waves of different polarizations propagating in the z direction experience similar surroundings and thus have similar dispersions as a result.

TABLE I. Empty lattice frequencies, in units of $2\pi/A$, at several high-symmetry points of rectangular lattices of different λ. The gap opening at these k points is crucial to the formation of a 3D full gap.

	N	**Γ**	**X***	**M**	**R**
$\lambda=\frac{2C}{A}$	$\frac{\sqrt{1+\lambda^2}}{2\lambda}$	$\frac{1}{\lambda}$	$\frac{\lambda^2-1}{2\lambda^2}$	$\frac{1}{\sqrt{2}}$	$\frac{\sqrt{1+2\lambda^2}}{2\lambda}$
10/7=1.43	0.610	0.7	0.745	0.707	0.789
10/8=1.25	0.640	0.8	0.820	0.707	0.812
10/9=1.11	0.673	0.9	0.906	0.707	0.838
10/10=1.00	0.707	1	1	0.707	0.866
10/11=0.91	0.743	1.1	1	0.707	0.896

The facts that $U_{\mathbf{G}_1}$ is dominating and that the corresponding TE and TM branches around $\mathbf{\Gamma}$ do not appreciably split up, make the local gap there the largest one—to the extent that other local gaps mostly fall within its gap frequencies (see Fig. 2). The formation of an absolute gap in a woven structure is, therefore, simplified to the alignment of the local gaps at **N**, **M**, and **R**—which favors the bcc one over the fcc structure as is clear from Table I. This explains why a full gap is developed in bcc [Fig. 2(b)] but not in fcc [Fig. 2(c)]. In our previous work,[13] we studied a simple rectangular woven structure made from a single kind of fibers. In that structure, a large gap at **Z** complicates the analysis and makes a large dielectric constant necessary for the gap opening. It is the use of different fibers in weaving (Fig. 1) that erases the complication at **Z** and leads to better properties.

In an attempt to optimize the conditions for gap opening, we find the best result in a system with $\lambda = 10/9$, which is slightly larger than the bcc structure ($\lambda = 1$). With this quasi-bcc structure, we are able to slightly increase the dimensions of the fibers (i.e., h and d). This leads to an increase in the packing fraction, which usually comes with enhanced scattering potentials $U_{\mathbf{G}}$'s and hence, wider band gaps.[2,13] In the present case, the enlarged packing fraction ($\sim 44\%$ of the volume) helps enlarging the gap size from **M** to **R** without much affecting the other bands. Thus, a wider full gap results. As shown in Fig. 2(d), the optimized result shows a full gap between 0.237 and 0.252 eV, which is about 7% of the gap center. Larger gaps have been discovered in several other 3D structures, but either the gaps are in lower frequency ranges[7] or the systems have to be fabricated by more complicated methods.[10] Considering the relative low packing fraction of this system,[6,18] we expect that there is much room for further improvement by simply enhancing the packing fraction and/or by employing a better fabric design. Best of all, by reducing the fiber dimensions to the submicron regime, we might even achieve a full gap in the optical range.

In summary, we have examined the formation of 3D absolute photonic band gaps in woven structures and have studied the associated gap properties. The analysis is generally applicable to other woven structures and other layered systems as long as there is a single outstandingly large scattering potential. In addition to the shape of the Brillouin zone, we found that the anisotropy of the dielectric distribution of the system is also crucial in opening an absolute gap. Our prediction for such systems is that a full gap could be more easily formed in a bcc, instead of a fcc structure, even though the latter might be favored in most other cases. One advantageous aspect of woven structures is that the weaving technology and fibers in microns are both available nowadays. Our calculations confirm that such systems, if properly designed, could have a 3D full gap in the infrared regime. We believe that the woven structures provide a way to realize the 3D photonic crystals in the infrared, and maybe even in the optical regimes.

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