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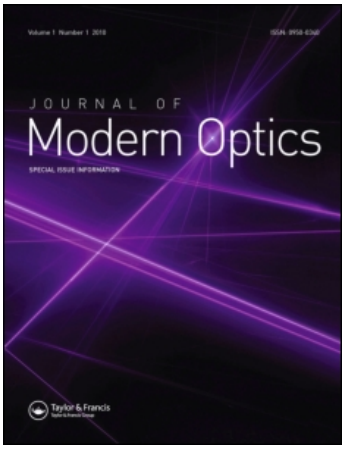

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Photonic Band Calculations for Woodpile Structures

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Photonic band calculations for woodpile structures

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Abstract. Photonic band structure has been computed for 'woodpile' structures having the periodicity of the simple tetragonal lattice. Bandgaps have been found. Further research directions are explored.

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1. Introduction

It has been some years now since Yablonovitch [2] and John [1] proposed that a periodic dielectric medium could prohibit the propagation of electromagnetic waves of certain frequencies in a manner similar to electronic band gaps in crystals. The idea was enthusiastically welcomed and since then numerous experimental and numerical studies have been published on the subject. The idea of a bandgap certainly applies to any wave equation, and indeed the band structure for neutron waves in a periodic magnetic field [15] and for sound waves [16] has also been explored. A more detailed account can be found in the review articles by Yablonovitch and Haus in this journal [14].

The search for structures that possess a photonic band gap has certainly had its twists and turns. The original suggestion was to explore periodic structures with a Brillouin zone (BZ) closest to a sphere. This was indeed an intuitively simple and sensible suggestion. Consequently, Yablonovitch and Gmitter [7] explored a structure which consisted of dielectric spheres placed at the lattice sites of the face centred cubic (f.c.c.) lattice, and the inverse structure where spherical voids were cut out of a high dielectric material. Although they reported a small bandgap between the second and third bands, calculations later revealed [8, 9, 10] that there was actually a degeneracy of the second and third bands at the W-point of the BZ, and hence that there was no gap. The degeneracy was so persistent that it was attributed to the symmetry properties of the W-point of the f.c.c. lattice and to the spherical symmetry of the 'atoms'.

Hence, John Maddox of *Nature* hastily proclaimed that photonic bandgaps had 'bitten the dust', thanks to the efforts of 'killjoy theoreticians'. Ironically, however, some of the very same structures that were investigated by Yablonovitch, namely structures with spherical voids in a dielectric background, did indeed have gaps, *not*

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between the second and third bands, where they were originally expected to appear, but between the eighth and the ninth [4, 6].

Ho *et al.* [10] reported band gaps in a structure where they placed a sphere at each lattice site in the diamond lattice, and also confirmed the same degeneracy at the *W*-point that had reported earlier. Later a structure with non-spherical atoms in f.c.c. was indeed demonstrated to possess large bandgaps [11]. Haus *et al.* also reported bandgaps [12] for structures where prolate spheroidal voids in a dielectric background were placed at the f.c.c. lattice points, with their symmetry axes oriented along the body diagonal of the unit cell. However, they showed that the bandgap opened only when the air spheroids overlapped. When the spheroids were isolated, even by a small amount, the gaps vanished. In an unpublished comment, they also pointed out that the 2–3 gap for dielectric spheres in the diamond lattice also disappeared when the sphere radius was even slightly reduced from its close-packed value, a finding which was later independently confirmed [5].

Although a number of different geometries were shown to possess bandgaps, these were structures that were difficult to manufacture even in the centimetre regime, and they stood little or no chance of being manufactured at micron sizes—although not for lack of trying. Noting that the appearance of the bandgap was closely related to the connectivity of the medium, Sözüer and Haus decided to experiment with various geometries in the simple cubic lattice in an effort to simplify the geometry and hopefully come up with a structure that could be scaled down to micron sizes. The result was a structure in which each point in the simple cubic lattice was connected to the six nearest neighbours with rods of circular cross-section. A related structure was one where the rods had a square cross-section. The latter structure had the advantage that it could be grown layer by layer using various deposition and lithographic techniques, whereas the circular rod structure did not allow such luxury. This structure was first presented at a workshop held in Utah in January 1992.

In March of the same year, Pendry and McKinnon submitted a manuscript to the *Physical Review Letters*, in which they detailed a novel numerical technique for calculating photonic band structures. To illustrate the utility of this new method, they calculated the photonic bands for a two-layer structure where metal rods were laid down parallel to the x-axis in one layer and in the second layer they were parallel to the y-axis. Repeating this pattern in the z-direction, one obtained a remarkably simple geometry. They calculated the band structure only for waves with the $\mathbf{k}$-vector in the z-direction, and hence it wasn't clear if this geometry would allow a photonic bandgap in all possible directions. Nevertheless, the idea was certainly novel, because the rods did not go 'through' each other, as the other studies suggested, but they were simply stacked up. This was especially useful because, by stacking up a set of rods in different ways, one could easily try out many structures. Unfortunately, the discussion on, and even the mention of, this structure was omitted in the published version of their paper [13] and hence never received proper attention.

This alternating-layers-of-rods structure was independently proposed by one of us (J.P.D.) during the course of discussions during a visit by H. S. S. to Alabama in January 1993. The basic idea seemed worthwhile to pursue and we also considered square rods arranged in a similar fashion. We loosely dubbed these 'woodpile' structures. Perhaps a more fair name could be 'Pendry–McKinnon structures' in recognition of the individuals who, to our knowledge, first suggested them.

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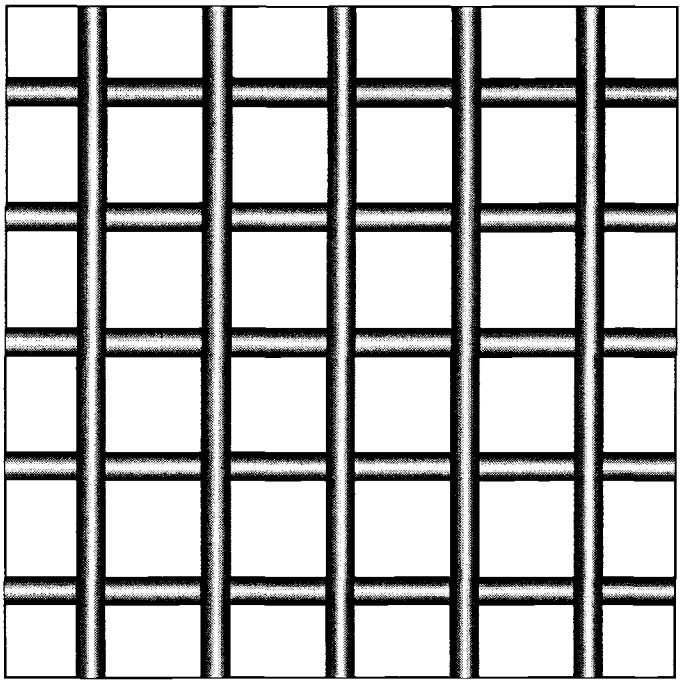

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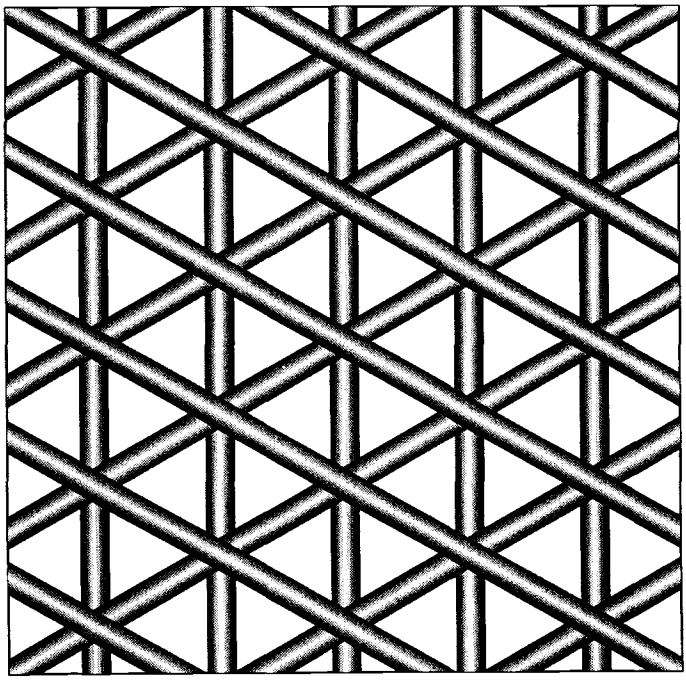

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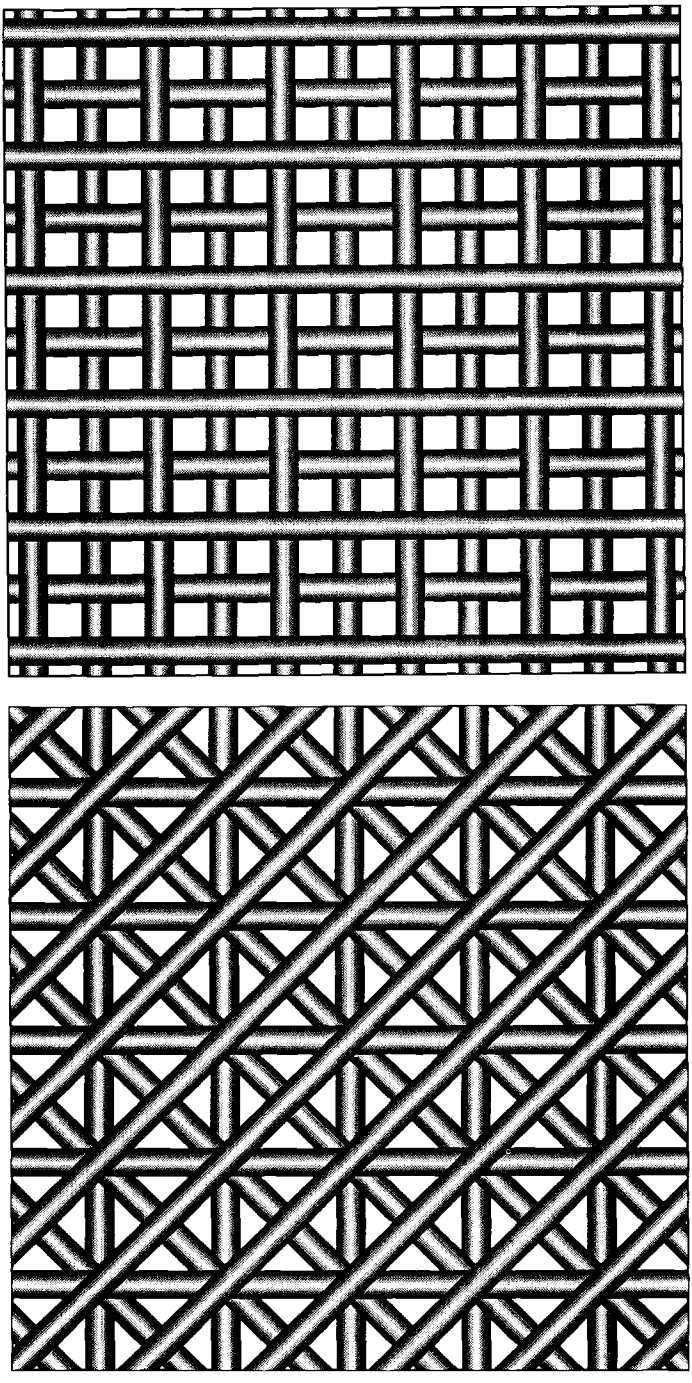

Figure 1. Improvisations on a basic theme. (*a*) The simple two-layer structure proposed by Pendry. (*b*) A three-layer 'screw' structure with the translational symmetry of the simple hexagonal lattice. Rods in each layer are rotated by 120° relative to the ones in the layer below. (*c*) A four-layer structure obtained from the simple tetragonal by shifting the third and the fourth layers rigidly by $(a_{xy}/2, a_{xy}/2)$ relative to the first two. This structure has the periodicity of the body centred lattice. (*d*) Another four layer structure where rods are rotated by 45° relative to the ones in the layer below.

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2. Method

We start with Maxwell's equations for $\mathscr{E}$ and $\mathscr{H}$ in a dielectric medium

$$\nabla \times \nabla \times \mathscr{E}(\mathbf{r}, t) + \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\epsilon(\mathbf{r})\mathscr{E}(\mathbf{r}, t) = 0, \tag{1}$$

$$\nabla \times \eta(\mathbf{r})\nabla \times \mathscr{H}(\mathbf{r}, t) + \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\mathscr{H}(\mathbf{r}, t) = 0, \tag{2}$$

where $\eta(\mathbf{r}) \equiv 1/\epsilon(\mathbf{r})$ and $\epsilon(\mathbf{r})$ is linear, locally isotropic, positive-definite and periodic with lattice vectors $\mathbf{R}$

$$\epsilon(\mathbf{r}) = \epsilon(\mathbf{r} - \mathbf{R}) > 0, \tag{3}$$

The eigenfunctions of equations (1) and (2) are Bloch functions of the form

$$\mathbf{E}_{n\mathbf{k}}(\mathbf{r}, t) = \exp[\mathrm{i}(\mathbf{k}\cdot\mathbf{r} - \omega_{n\mathbf{k}}t)]\sum_{\mathbf{G}}\mathbf{E}_{n\mathbf{k}}(\mathbf{G})\exp[\mathrm{i}(\mathbf{G}\cdot\mathbf{r})] \tag{4}$$

$$\mathbf{H}_{n\mathbf{k}}(\mathbf{r}, t) = \exp[\mathrm{i}(\mathbf{k}\cdot\mathbf{r} - \omega_{n\mathbf{k}}t)]\sum_{\mathbf{G}}\mathbf{H}_{n\mathbf{k}}(\mathbf{G})\exp[\mathrm{i}(\mathbf{G}\cdot\mathbf{r})] \tag{5}$$

where $\mathbf{G}$ is a reciprocal lattice vector and the Fourier coefficients $\mathbf{E}_{\mathbf{G}} \equiv \mathbf{E}_{n\mathbf{k}}(\mathbf{G})$ and $\mathbf{H}_{\mathbf{G}}$ satisfy, respectively, the infinite-dimensional matrix equations

$$(\mathbf{k}+\mathbf{G}) \times [(\mathbf{k}+\mathbf{G}) \times \mathbf{E}_{\mathbf{G}}] + \frac{\omega^2}{c^2}\sum_{\mathbf{G}'}\epsilon_{\mathbf{G}\mathbf{G}'}\mathbf{E}_{\mathbf{G}'} = 0, \tag{6}$$

$$(\mathbf{k}+\mathbf{G}) \times \left[\sum_{\mathbf{G}'}\eta_{\mathbf{G}\mathbf{G}'}(\mathbf{k}+\mathbf{G}') \times \mathbf{H}_{\mathbf{G}'}\right] + \frac{\omega^2}{c^2}\mathbf{H}_{\mathbf{G}} = 0, \tag{7}$$

with $\epsilon_{\mathbf{G}\mathbf{G}'} \equiv \epsilon(\mathbf{G} - \mathbf{G}')$ and $\eta_{\mathbf{G}\mathbf{G}'} \equiv \eta(\mathbf{G} - \mathbf{G}')$. Equation (6) is an infinite-dimensional generalized Hermitian eigenproblem, hereafter referred to as the E method, while equation (7) is an ordinary one, which we will call the H method. The Bloch functions satisfy the following orthogonality relations [4]

$$\int_{\text{all } \mathbf{r}} \mathrm{d}\mathbf{r} \exp[-\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}]\epsilon(\mathbf{r})\mathbf{E}^*_{n'\mathbf{k}'}(\mathbf{r})\cdot\mathbf{E}_{n\mathbf{k}}(\mathbf{r}) = C_{n\mathbf{k}}\delta_{nn'}\delta(\mathbf{k}-\mathbf{k}'), \tag{8}$$

$$\int_{\text{all } \mathbf{r}} \mathrm{d}\mathbf{r} \exp[-\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}]\mathbf{H}^*_{n'\mathbf{k}'}(\mathbf{r})\cdot\mathbf{H}_{n\mathbf{k}}(\mathbf{r}) = C'_{n\mathbf{k}}\delta_{nn'}\delta(\mathbf{k}-\mathbf{k}'), \tag{9}$$

where $\{C_{n\mathbf{k}}\}$ and $\{C'_{n\mathbf{k}}\}$ are real and positive normalization constants. It is important to note that the $\mathscr{E}$ field is normalized with $\epsilon(\mathbf{r})$ as the weight function. Although the two formulations, the E and the H method, would yield the same spectrum when an infinite number of plane waves are included, their truncated forms yield, in general, very different spectra even when as many as a few thousand plane waves are used.

Using $\nabla \cdot \nabla \times \mathscr{E} = 0$ and $\nabla \cdot \mathscr{H} = 0$, the $3N \times 3N$ matrix equations (6) and (7) can be cast into $2N \times 2N$ ordinary Hermitian forms which are computationally more efficient. Hence the E method is identical to the method of Ho *et al.* [10], while the H method uses the same matrix equation with $\tilde{\epsilon}^{-1}_{\mathbf{G}\mathbf{G}'}$ replaced by $\eta_{\mathbf{G}\mathbf{G}'}$.

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Following Zhang and Satpathy [9], one could also start with the equation satisfied by the $\mathscr{D}$ field,

$$\nabla \times \nabla \times \eta(\mathbf{r}, t) + \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\mathscr{D}(\mathbf{r}, t) = 0. \tag{10}$$

This was shown to be equivalent to the H method [4].

The periodic dielectric function is written as

$$\epsilon(\mathbf{r}) = \epsilon_b + \sum_{\mathbf{R}} \epsilon_0(\mathbf{r} - \mathbf{R}). \tag{11}$$

where ϵ_b is the dielectric constant of the 'background' and $\mathbf{R}$ is a lattice vector. Its Fourier transform (FT) is

$$\begin{aligned}\epsilon(\mathbf{G}) &= \frac{1}{V_{\text{cell}}} \int_{WS\,\text{cell}} d\mathbf{r} \exp(-i\mathbf{G}\cdot\mathbf{r})\epsilon(\mathbf{r}), \\ &= \epsilon_b \delta_{\mathbf{G}0} + \frac{1}{V_{\text{cell}}} \int_{\text{all}\,\mathbf{r}} d\mathbf{r} \exp(-i\mathbf{G}\cdot\mathbf{r})\epsilon_0(\mathbf{r}),\end{aligned} \tag{12}$$

and a similar expression holds for $\eta(\mathbf{G})$.

The lowest order Fourier expansion for each method yields the two possible extreme limits for the effective long-wavelength dielectric constant ϵ_{eff}. This gives the methods a complementary nature, since, as the number of plane waves used in the expansion is increased, they approach a common limit from two extreme starting points.

3. Results

The recipe for building the structure proposed by Pendry was simple enough: place wires separated by a certain distance all parallel to the x axis; place another layer on top of the first, but this time with the wires parallel to the y axis; repeat. There are many improvisations on this structure that can readily be made. The most obvious is to use wires of rectangular cross-section. This is particularly relevant if one is contemplating producing these at micron sizes, since flat surfaces are much easier to produce than rounded ones. Another issue is how many distinct layers one stacks up in the z direction. Indeed, there are many possibilities, some of which are displayed in figure 1.

For each one of the structures displayed, there are a number of geometrical parameters that need to be varied and consequently the problem can easily become overwhelming. One's natural instinct is to try out the simplest one, namely the two layer structures first, which is what we did. We kept the x and the y axes equivalent, although one could, of course, make the two different by placing different rods along, say, the y axis or by changing the interrod spacing. The z direction, however, is distinct and hence these are uniaxial structures. $\epsilon(x, y, z)$ is invariant under the permutation of x and y, i.e., $\epsilon(x, y, z) = \epsilon(y, x, z)$. In addition, $\epsilon(x, y, z)$ has mirror symmetry about the xy, yz and zx planes, i.e., $\epsilon(x, y, z) = \epsilon(-x, y, z)$, etc. Consequently, there are 16 symmetry operations that leave $\epsilon(x, y, z)$ invariant. An immediate result of this is that the non-repeating portion of the BZ is three times larger than one would have with spherical atoms in a lattice with cubic symmetry.

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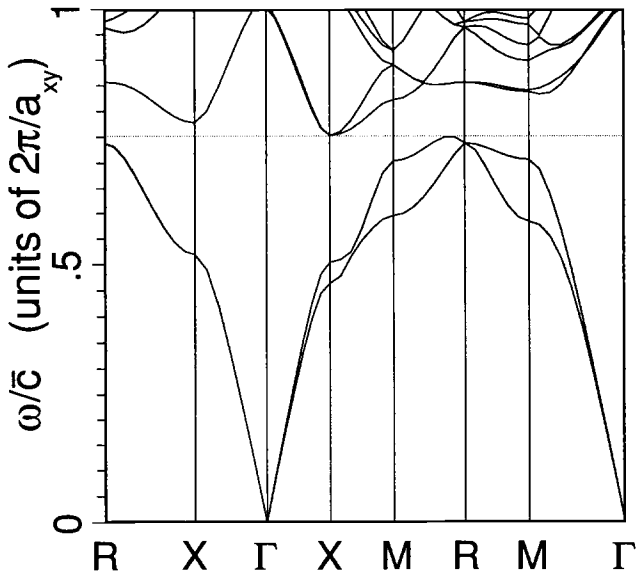

Figure 2. The photonic band structure for 'close-packed' circular rod structure. $\epsilon_b = 1$, $\epsilon_a = 16$, $R_c = 1{\cdot}4$ and $a_z = 5{\cdot}6$. All lengths are in units of $a_{xy}/2\pi$. The bandgap shown is only half a per cent.

3.1. *Circular rods*

The dielectric function for circular rod structures is expressed as in equation (11) with

$$\epsilon_0(\mathbf{r}) = (\epsilon_a - \epsilon_b)[\theta(a_{xy}/2 - |x|)\theta(R_c - \rho_{yz}) + \theta(a_{xy}/2 - |y|)\theta(R_c - \rho_{z'x})], \tag{13}$$

where R_c is the radius of the cylinders, $a_{xy} \equiv a_x = a_y$ and a_z are the sides of the tetragonal unit cell along the x, y and the z directions, $\rho_{yz} \equiv (y^2 + z^2)^{1/2}$, and $\rho_{z'x} \equiv [(z - a_z/2)^2 + x^2]^{1/2}$. The Fourier transform of $\epsilon(\mathbf{r})$ is then written as

$$\epsilon(\mathbf{G}) = \epsilon_b \delta_{\mathbf{G}0} + (\epsilon_a - \epsilon_b)\frac{\pi R_c^2 a_{xy}}{V_{\text{cell}}}\left[\frac{2J_1(G_{yz}R_c)}{G_{yz}R_c}\delta G_x 0 + \frac{2J_1(G_{zx}R_c)}{G_{zx}R_c}\delta_{G_y 0}\cos\left(G_z\frac{a_z}{2}\right)\right], \tag{14}$$

where $J_1(x)$ is the first order Bessel function, $G_{yz} \equiv (G_y^2 + G_z^2)^{1/2}$, $G_{zx} \equiv (G_z^2 + G_x^2)^{1/2}$, and the cosine factor arises from the displacement of the axis of the rods parallel to the y axis.

In figure 2 we plot the band structure for cylinders with $\epsilon_a = 16$ in an air background. The bandgap is rather small although it tended to increase somewhat as the Fourier basis was increased. The band structure with cylindrical holes was highly anisotropic at the volume fractions necessary to obtain a gap, and hence did not possess any gaps.

3.2. *Rectangular rods*

We also tried using rectangular rods of width $2R_{xy}$ and height $2R_z$ placed in a similar manner. The dielectric function for this structure is expressed as in equation (11) with

$$\begin{aligned}\epsilon_0(\mathbf{r}) = (\epsilon_a - \epsilon_b)[&\theta(a_{xy}/2 - |y|)\theta(R_{xy} - |x|)\theta(R_z - |z|) \\ &+ \theta(a_{xy}/2 - |x|)\theta(R_{xy} - |y|)\theta(R_z - |z - a_z/2|)].\end{aligned} \tag{15}$$

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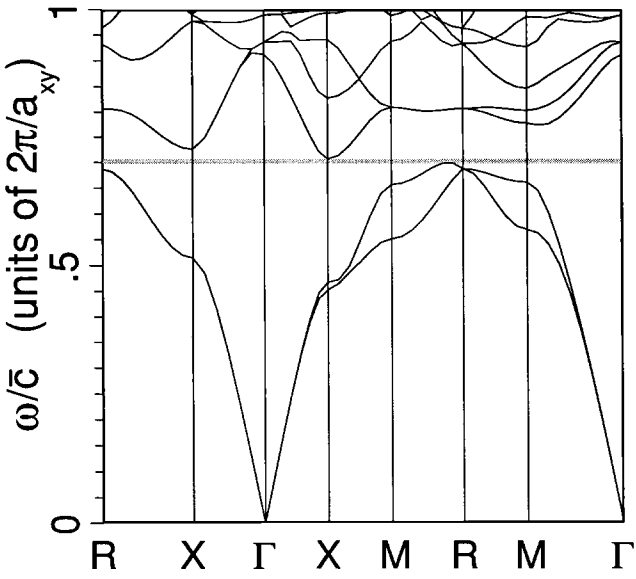

Figure 3. The photonic band structure for 'close-packed' rectangular-rod structure. $\epsilon_b = 1$, $\epsilon_a = 16$, $R_{xy} = 0{\cdot}75$, $R_z = 1{\cdot}4$ and $a_z = 5{\cdot}6$. All lengths are in units of $2\pi/a_{xy}$. The bandgap shown is 2–3%.

Again, the rods parallel to the y axis are displaced by $(0, 0, a_z/2)$ relative to the origin. The FT of $\epsilon(\mathbf{r})$ is

$$\epsilon(\mathbf{G}) = \epsilon_b \delta_{\mathbf{G}0} + (\epsilon_a - \epsilon_b) \frac{a_{xy}(2R_{xy})(2R_z)}{V_{\text{cell}}} \left[\frac{\sin Y}{Y} \frac{\sin Z}{Z} \delta_{G_x 0} + \frac{\sin Z}{Z} \frac{\sin X}{X} \delta_{G_y 0} \cos\left(G_z \frac{a_z}{2} \right) \right], \tag{16}$$

where $X \equiv G_x s/2$, $Y \equiv G_y s/2$, $Z \equiv G_z s/2$ and $V_{\text{cell}} = (2\pi)^3$ is the volume of the simple cubic (s.c.) unit cell.

This structure is interesting also because its topology is the same for all values of β. Furthermore, the a- and the b-type regions, except for size, have exactly the same geometry and for $\beta = 0{\cdot}5$ the two regions are identical. β again refers to the volume fraction of the a-type material. In fact the topology of both of these structures is identical to the scaffold structures described in [3].

After trying a large region of filling fractions and aspect ratios we found gaps of size 2–3% with a dielectric constant of 16. We also tried making a_z larger than its close-packed value of $a_z = 4R_z$ but still the size of the gaps did not increase much. Although at any given point of the BZ the separation of the bands is large, the forbidden bands at the X and the R points overlapped only by a small amount. With a dielectric constant of 25, the gaps increased significantly to approximately 7–10%.

4. Discussion

We have shown that the two-layer woodpile structures do have bandgaps, but with ordinary semiconductors with refractive indices of 3·5–4, the gaps are too small to be truly useful. We are currently exploring more complex structures with more than two layers. Our preliminary calculations with the four-layer structure have shown gaps of over 20%.

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Acknowledgments

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