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Three-dimensional photonic band gaps in woven structures

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Abstract. In this paper, we studied the photonic properties of dielectric fibres woven into three-dimensional (3D) structures. Such fibres can be fabricated on the micrometre scale, and hence the gaps are in the far-infrared to the infrared regime. The vector-wave transfer matrix method is applied to evaluate the photonic band structures. We have also employed the constant-frequency dispersion surface scheme to investigate the development of a full band gap. Such a 3D absolute gap is observed in a rectangular lattice, but at a fairly large dielectric constant for the fibres. Ways to improve on this have been suggested. Our study indicates that woven structures are promising materials for realizing the 3D photonic insulator in the infrared regime.

1. Introduction

The formation of electronic bands in periodic potentials has been known of for decades. Recently, it has been reported that periodic dielectric materials can introduce similar band phenomena to electromagnetic (EM) waves [1, 2]. Inside a so-called photonic band gap (PBG), the scattering of EM waves by the dielectric materials becomes destructive and leads to a complex wave vector; i.e. the wave field decays exponentially therein [3]. Therefore, there will be no propagating mode in the gap region if the materials are thick enough. The formation of a PBG could cause several new phenomena in quantum electrodynamics [4, 5]. Its possible applications such as suppressing the spontaneous emission and improving the quality of optical devices have also been intensively studied [1, 6]. However, due to the complicated vector nature of the EM waves, the bands of different polarizations are generally non-degenerate and a common gap is difficult to find. Although PBGs have been reported to occur in many artificial systems, most of their gaps exist only in limited directions, i.e. the propagation of EM waves is forbidden in some directions but allowed in others [2, 6]. This implies that a slight change of the angle of incidence may cause the 'leakage' of the EM waves. It is therefore important to find a structure with an absolute gap, i.e. a photonic insulator which, within a certain frequency range, allows no EM propagation in *any* direction.

There exist several successful two- and three-dimensional (2D and 3D) photonic insulators fabricated by means of the etching techniques which were developed for semiconductors in the millimetre regime; the gaps so obtained were in the microwave range [6–10]. It is desirable to have PBG in the infrared or the visible frequencies which are the frequency ranges for most lasers and thus have important application possibilities.

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To achieve this, the lattice size of the photonic system has to be reduced, by the scaling law, to the micrometre scale, which is very difficult with current etching techniques. Various methods of fabrication were proposed such as chemically assisted ion-beam etching [11], holographic techniques [12] and other combined methods [13], but so far only 2D photonic gaps at these frequencies have been obtained in this way [12, 14]. Forming 3D absolute photonic band gaps remains a task to be achieved.

Here in this paper, we propose a woven structure which is composed of dielectric fibres woven into layers of identical patterns. The layers are then stacked one upon another to produce a 3D-lattice structure. Fibres with cross sections in micrometres have been available for years, especially since the launch of the optical fibre communications [15]. Weaving technology for fine fibres has also been known of for centuries; for example, silk fibres can be woven into materials that show diffraction effects as is evident when an umbrella is held up to street lights. The key point is that fibres can be woven on a relatively open scale with low-technological techniques and subsequently form a fine pattern whose scale is limited only by the dimensions of the fibres themselves. This is a unique property of a woven structure. Other structures require assembly on a scale to match the target wavelength. Our study indicates that fibres woven into a rectangular lattice can indeed have a full 3D photonic band gap in the mid-infrared regime. In fact, the structure that we identify will work as a photonic insulator at any wavelength provided just that (1) the scale of the structure can be adjusted to match the incident wavelength and (2) a suitable fibre can be found with large enough dielectric constant ($\epsilon \geqslant 40$ in our case). Though there are difficulties in realizing the latter condition at optical wavelengths, it is easily achieved for longer wavelengths. For example, single-crystal tellurium (Te) as the core material for optical fibres has diffraction indices equal to 4.9 and 6.3 for the two polarizations at 4 μm [15, 16]. Meanwhile, there are ways to reduce the dielectric constant of the fibres, such as employing more compact lattice structures. This will be discussed later.

This paper is organized as follows. In section 2, the details of woven structures are given and the vector-wave transfer matrix method [17] is applied to study their band structures. In section 3, we analyse the calculated band structures and employ the constant-frequency dispersion surface scheme [18] to further examine the completeness of the gap formation. A brief summary is given in section 4.

2. Woven structures and the transfer matrix

The unit cell of the woven structure considered in this paper is composed of four identical fibres with dielectric constant ϵ_w and diameter d, which are woven into a hash-like pattern as shown in figure 1. The whole system is embedded in a background medium with dielectric constant ϵ_b (here assumed to be vacuum). The centre-lines of the fibres in one unit cell are given by

$$\left(x, \pm\frac{A}{4}, \pm h \sin\left(\frac{2\pi}{A}x\right)\right) \qquad \text{and} \qquad \left(\pm\frac{A}{4}, y, \mp h \sin\left(\frac{2\pi}{A}y\right)\right). \tag{1}$$

A is the lattice constant in both the x- and y-directions, and h is the amplitude of the variation of the centre-line in the z-direction. To support and to separate the woven layers, a uniform dielectric slab with dielectric constant ϵ_s is inserted between every two of them. The thickness of the slab is $C - 2h - d$, where $C = \lambda A$ is the lattice constant in the z-direction. Note that λ can be any number, i.e. the unit cell is, in general, rectangular. Unit cells are then stacked up to form a 3D lattice. If the stacking of the layers has perfect alignment, the lattice has the simple rectangular structure. Alternatively, if $C = A$, we may

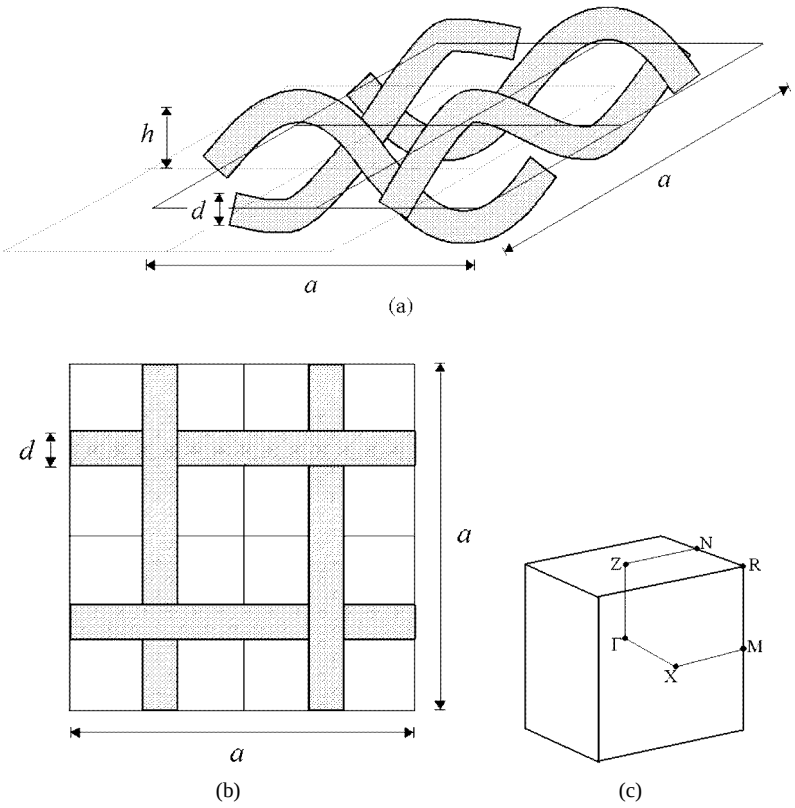

Figure 1. (a) The unit cell of a woven structure, where fibres are curved in sine-wave forms; (b) the top view of the unit cell; (c) the first Brillouin zone of the woven structure.

have either the bcc or the fcc structure depending on how the layers are aligned. Here we consider the simple rectangular case.

In the following studies, we employ the vector-wave transfer matrix method developed from low-energy electron diffraction [17], which has been successfully applied in calculating the photonic band structures of periodic dielectric systems [17, 19]. The basic concept of this method is that of discretizing Maxwell's equations

$$\nabla \times \boldsymbol{E} = -\mu\mu_0 \frac{\partial \boldsymbol{H}}{\partial t} \qquad \nabla \times \boldsymbol{H} = -\epsilon\epsilon_0 \frac{\partial \boldsymbol{D}}{\partial t} \tag{2}$$

on a lattice so that the propagation of the $\boldsymbol{E}$- and $\boldsymbol{H}$-fields through the material can be determined with the transfer matrix formalism. Take the z-direction EM-wave propagation, for example. The unit cell is first sliced into layers of thickness c. The EM wave at $z = c$ can be expressed in terms of the field in the $z = 0$ plane; i.e.

$$\boldsymbol{F}(\rho, c) = \sum_{\rho'} \mathbf{T}(\rho, c; \rho', 0)\boldsymbol{F}(0) \tag{3}$$

where

$$\boldsymbol{F}(\boldsymbol{r}) = \begin{pmatrix} E_x(\boldsymbol{r}) \\ E_y(\boldsymbol{r}) \\ H_x(\boldsymbol{r}) \\ H_y(\boldsymbol{r}) \end{pmatrix}$$

where $\boldsymbol{r} = (\rho, c)$, and $\mathbf{T}$ is the transfer matrix connecting two adjacent planes. The EM field is then integrated slab by slab and finally the effective transfer matrix for a unit cell is obtained. This means that given the wave field on one side of a unit cell, we can calculate the field on the other side. The calculation of the wave propagation in other directions can be performed similarly. Details of this method can be found in references [17] and [19].

For periodic systems, the Bloch band theory is applicable:

$$\exp(\mathrm{i}k_z C)\boldsymbol{F}(z) = \boldsymbol{F}(z + C) \tag{4}$$

where C is the lattice constant in the z-direction. At given k_x and k_y, equations (3) and (4) together form an eigenvalue problem for the $\mathbf{T}$ matrix, which determines the dispersion, $k_z(\omega)$. In this way, we can calculate the band structure, or the dispersion $\boldsymbol{k}(\omega)$, for any $k = (k_x, k_y, k_z)$. In short, the transfer matrix method enables us to study the photonic band structure, in which the Bloch wave vector $\boldsymbol{k}$ along the EM-wave incidence direction is determined at a given frequency ω.

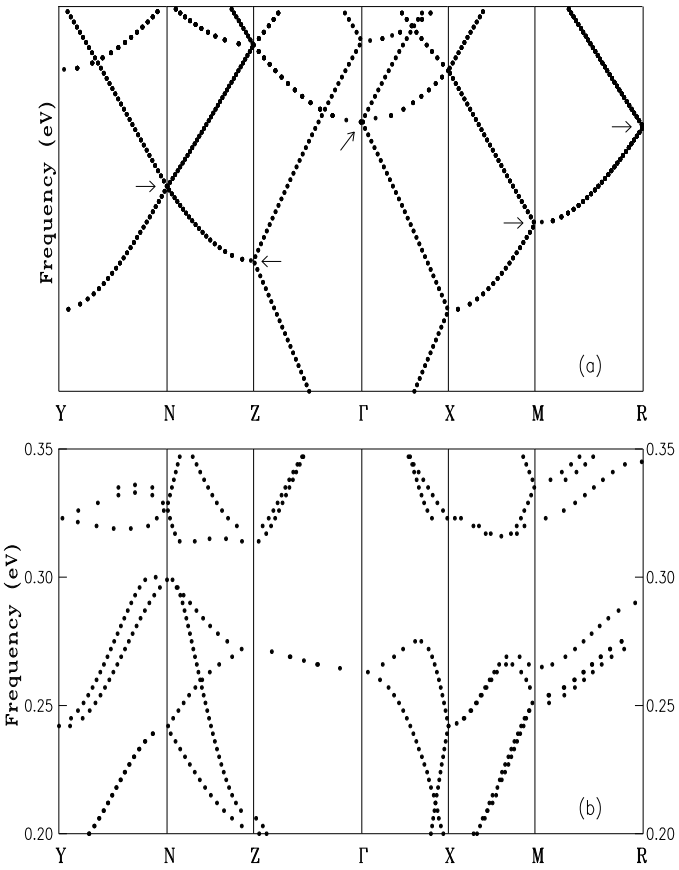

Figure 2. The calculated band structures of (a) an empty lattice and (b) a rectangular woven lattice, where $A = 1.87$ μm, $h = 0.16A$, $d = 0.13A$, $\epsilon_w = 40$, $C = 0.8A$ and $\epsilon_s = 1.0$, i.e. the slabs are assumed identical to the background. The packing fraction of the fibres is 7.7% and a full gap between 0.302 and 0.309 eV is observed in (b).

3. Photonic band structures for the woven systems

Figures 2(a) and 2(b) show the band structures determined with the transfer matrix method for an empty lattice and a rectangular woven system, respectively. The two systems have the same geometric structure, but ϵ_w is set to 1 for the empty lattice. The woven system is invariant under the C_4 rotation about the z-axis, which leads to zero gaps at the first Brillouin zone boundaries along the k_x- and k_y-directions (see figure 2(b)). One can also examine the Fourier components of the dielectric function, U_{nG_x} and U_{nG_y}, where G_x (G_y) is $2\pi/A$. These two components are approximately proportional to the gap sizes at $k = nG_x$ or nG_y, respectively [3, 20]. The calculations show that U_{nG_x} and U_{nG_y} are non-vanishing only when n is even; i.e. $n = 2$ for the first gap in the x- and y-directions. One obvious choice for an absolute band gap is thus located in the $n = 2$ gap region. In order to bring the first z-direction gap into this frequency range, one might expect to have a smaller z-direction lattice constant at $C \simeq 0.5A$ (i.e. $\lambda \simeq 0.5$). However, we have more to consider. Arrows in figure 2(a) indicate the zone boundaries where we wish to open gaps and align them for an absolute band gap for the system. Having $\lambda = 0.5$ would be unfavourable as regards that aim, since we would still like to keep the Brillouin zone as close to a sphere as possible [7]. For example, the R point in the Brillouin zone (see figure 2(c)) is located at a distance $(\sqrt{1 + 2\lambda^2}/2\lambda)\, 2G_x$ from the Γ point and will be close to the $2G_x$-gap at the X point if $\lambda \simeq 0.7$.

Further complications arise from there being many degenerate bands in the empty-lattice case (figure 2(a)), which become non-degenerate after the Bloch scattering is taken into account (figure 2(b)); i.e. U_G is polarization dependent. The effect of polarization is most clearly seen around the X point, for the reason that the dielectric functions are highly asymmetric for EM waves of different polarizations travelling in the x-direction. This phenomenon hinders us from obtaining the absolute gap since gaps of the two polarizations usually do not overlap considerably. Therefore, reducing the polarization-dependent difference in the dielectric function at certain k-points is important. Taking all of these points into consideration, we found that corner points like R and N are most crucial to the development of an absolute band gap in a rectangular woven structure, and the optimal λ-value is at $\sim$0.8.

Figure 2(b) is calculated with $A = 1.87$ μm, $h = 0.16A$, $d = 0.13A$, $\epsilon_w = 40$, $\epsilon_s = 1.0$ and $\lambda = 0.8$. As can be clearly seen, a full gap is indeed developed between 0.302 and 0.309 eV, the width of which is approximately 2.3% of the gap-centre frequency. Note that the gap is located in the mid-infrared regime. On the experimental side, full gaps of much larger size have been observed in different frequency ranges for different systems [7, 10]. We note, however, that gap positions are generally difficult to locate accurately with finite-sized samples in transmission measurements [3]. In order to further examine the completeness of the 3D gap, we have also employed the so-called dispersion surface scheme [18]. Here we calculate the dispersion $k_z(\omega)$ as a function of (k_x, k_y) at a fixed frequency and obtain a constant-frequency surface in k-space. This is similar to the formation of the Fermi surface in the electronic cases. For a uniform dielectric system, the constant-frequency surface for EM waves is a degenerate sphere (for the two polarizations) with the radius $\omega\sqrt{\epsilon}/c_0$ where c_0 is the speed of light. In this case, the sphere exists for all frequencies, i.e. there is no gap anywhere. When the periodic dielectric function is introduced, the Bloch scattering causes distortion of the constant-frequency spheres and the two polarizations become non-degenerate. The distortion is most pronounced near the Brillouin zone boundaries where bands must intersect at right angles [18, 20]. A band gap shows up in the dispersion surface calculation when $k_z(\omega)$ is absent over a certain frequency range. If the absence of $k_z(\omega)$

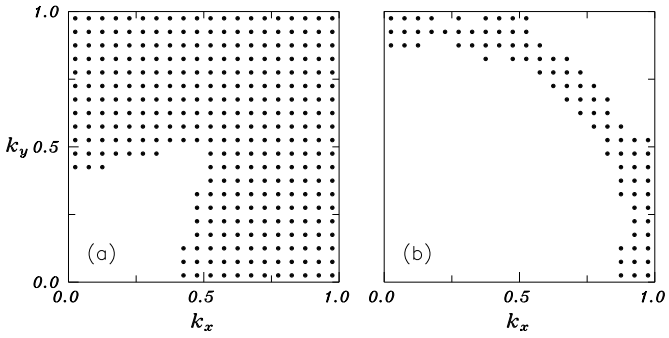

Figure 3. The projections of dispersion surfaces for two rectangular woven systems, where the empty space denotes the forbidden region. These systems have the same geometric structure: $A = 1.87$ μm, $h = 0.15A$, $d = 0.13A$ and $C = 0.8A$. The slabs are assumed to be composed of the same material as the background and the packing fraction of the fibres is 7.7%. The dielectric constants of the wires, ϵ_w, are (a) 20 and (b) 30. When ϵ_w reaches 40, a 3D absolute gap is fully developed and the whole Brillouin zone becomes empty.

becomes persistent throughout the k_x–k_y plane, an absolute band gap can be identified.

Figure 3 shows the projections of the calculated dispersion surfaces on the k_x–k_y plane for two rectangular woven systems which are identical to the one in figure 2(b), but with smaller ϵ_ws ($\epsilon_w = 20$ for figure 3(a) and 30 for figure 3(b)). The energies are chosen to fall within the first gap at the N point of the corresponding band structures (see figure 2(b)). Dots in the figure indicate the presence of allowed modes in the frequency range. Since we are looking for an absolute gap, there is no need to distinguish between the polarizations. Meanwhile, only the first quadrant of the Brillouin zone is shown since the systems possess C_4 symmetry. The empty region in the lower left-hand corner corresponds to the gap opened at the $k_z = \pm G_z/2$ boundaries. When ϵ_w is increased from 20 to 30, the allowed modes are driven to a more restricted region as the empty region grows (see figure 3(b)). Eventually, when ϵ_w reaches 40, the dispersion surface becomes so distorted that the allowed modes are all expelled from the 2D Brillouin plane, indicating the formation of a full 3D photonic gap in the infrared regime.

Dielectric constants as large as 40 may not be very practical to use. However, there is room for improvement. Consideration of how to reduce the dielectric constant of the fibre while achieving a 3D absolute photonic band gap is given below. It should also be noted that, on altering the lattice design, the frequency range in which the gap locates may also be easily adjusted. The dielectric modulation, which determines the gap sizes, is approximately proportional to the Fourier component of the dielectric function:

$$U_G = \frac{1}{v_c} \int_{\text{cell}} [\epsilon_b + (\epsilon_w - \epsilon_b)\rho(\boldsymbol{r})]\, \mathrm{e}^{-\mathrm{i}\boldsymbol{G}\cdot\boldsymbol{r}}\, \mathrm{d}^3 r \tag{5}$$

where $\rho(\boldsymbol{r})$ is the distribution function of the fibres. The packing fraction, f, is given by the ratio between the region where $\rho(\boldsymbol{r}) \neq 0$ and the total volume. In certain cases, where the 'atoms' are carved out from a uniform background material [7], equation (5) still holds, but f may then be better referred to as the removed packing fraction. It is clear from equation (5) that there are two ways to modify the dielectric modulation for a wider gap: by enhancing the dielectric contrast between the fibres and the background materials, or by increasing the packing fractions. In general, the gap size grows wider with f until the latter reaches an optimal value, beyond which the gap width starts to decrease. This is because

the dielectric modulation decreases when the fibres occupy too much space in the unit cell, and becomes more and more uniformly distributed [3]. Note that local gaps at different k-points vary differently as f changes and thus the overall optimal f for the widest possible absolute gap of the system has to be determined from the details of the band structures. The packing fraction of the rectangular woven structure under study is rather small (∼8%), and thus has much room for improvement. In comparison, it takes large removed packing fractions of 60–70% to open a full gap in reference [7].

The packing fraction of the woven structure is mainly determined by the amplitude h and the diameter d of the fibres, where the latter is more important since $f \propto d^2$. For a rectangular lattice, since h and d have to satisfy the relation $d/2 < h < C/2 - d/2$, even the maximum packing fraction is still rather small (∼25%). This implies that the dielectric modulations may be enhanced by employing more compact lattice structures like bcc or fcc, for which f can be as large as ∼45% and the Brillouin zones are closer to spheres. Then, it would be possible to reduce the dielectric constant of the fibres but still retain large dielectric modulations for an absolute gap. However, complications do arise in these cases—for example, due to the symmetry of the systems and the polarization dependence of the gap positions. More studies are obviously needed to identify the optimal design of the woven materials to be employed in a photonic system. Our study on the bcc structure shows that, for example, one such problem, due to the symmetry of the woven layer, can be eliminated by weaving two kinds of fibre in the structures [21]. Preliminary calculations also show that the dielectric constants of the fibres can be significantly reduced to moderate values while an absolute gap remains. This is a strong indication that a 3D absolute photonic gap could be realized with the use of a carefully designed woven structure. Further detailed results will be reported elsewhere [21].

4. Summary

In this paper, we have proposed and discussed a simple and yet feasible photonic system of woven structures. The system is composed of fibres on the micrometre scale and can be fabricated with currently available weaving techniques. We have studied its photonic band structures by the well-established transfer matrix method. The band structures are complicated by the symmetry of the system and the polarization dependence of the Bloch scatterings and, hence, a rectangular structure is preferred to a cubic one. With the help of the constant-frequency dispersion surface scheme, we have also examined how an absolute gap is developed. Our calculations show the existence of an absolute gap in the rectangular structure even though the packing fraction can be as small as 10%. This result has an important implication: with the employment of more compact structures, an absolute 3D gap may possibly be achieved by using fibres of moderate dielectric constants. Woven structures seem promising for realizing a 3D photonic insulator in the infrared regime.

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