Photonic band gaps in two-dimensional square lattices: Square and circular rods

Pierre R. Villeneuve and Michel Piché
Centre d'Optique, Photonique et Laser, Département de Physique, Université Laval, Québec, Québec, Canada G1K 7P4
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Periodic arrays of rods with either a square or circular cross section located at the corners of a square lattice exhibit photonic band gaps common to s and p polarizations. The overlap of s and p gaps is generated in arrays of low-index rods embedded in a dielectric background of higher index. The overlap does not occur between the same bands in arrays of rods with a square cross section and a circular cross section. Arrays of rods with a circular cross section require a lower index contrast to generate a band gap than rods with a square cross section, but do not necessarily yield larger gaps at higher index contrasts.

It has been proposed[1,2] that dielectric structures with a periodic index of refraction could give rise to photonic band gaps for which propagation of electromagnetic waves would be forbidden in the periodic structure. Such band gaps are characterized by a separation of the bands across all symmetry points of the Brillouin zone for orthogonal polarizations. The existence of such band gaps in some structures with three-dimensional lattices has been shown theoretically[3] and experimentally.[4] In three-dimensional lattices, the band diagrams for both polarizations are very similar and many of these bands are degenerate (at least at the symmetry points), hence, the gaps are likely to overlap. On the other hand, the band diagrams for orthogonal polarizations in structures with two-dimensional lattices are very different. As a consequence, the gaps are not as likely to overlap. It has been shown,[5–7] however, that periodic arrays of rods can give rise to band gaps common to both polarizations in the plane perpendicular to the rods; in particular, it has been shown that structures with either hexagonal[6,7] or square[6] lattices can generate such band gaps.

In this paper, we investigate the effects of the cross-sectional geometries of the rods in a square lattice. The structure consists of an array of long parallel rods of either square or circular cross section whose centers form a square lattice in the plane perpendicular to the rods. Such square lattices are ideal for the analysis of square and circular rods, since their filling fraction can be quite large before reaching the close-packed condition; when the filling fraction is greater than the close-packed limit, the rods overlap and the structure is no longer self-supporting. The close-packed condition is reached when the filling fraction is 79% if the cross section of the rods is circular and 100% if the cross section is square. In both structures, band gaps occur when the filling fractions are under the close-packed limit. The refraction index of the background material may be greater or less than that of the rods. Although the material of low index need not be air, we will refer to dielectric-air structures for simplicity.

The electric field propagating in the periodic plane can be expanded in a series of plane waves of the form

$$\mathbf{E}(x,y,t)=e^{i\omega t}\sum_{j=1}^{3}\sum_{\mathbf{G}} A_{\mathbf{G},j}\hat{\mathbf{e}}_j e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}\ , \tag{1}$$

where $\mathbf{k}$ is the wave vector and $\mathbf{G}$ the reciprocal-lattice vector. Maxwell's equations can then be reduced to two standard eigenvalue equations. When the electric field is parallel to the rods (s polarization), Maxwell's equations become

$$\sum_{\mathbf{G}'}|\mathbf{k}+\mathbf{G}-\mathbf{G}'|^2 d_{\mathbf{G}'}A_{\mathbf{G}-\mathbf{G}',3}-\omega^2 A_{\mathbf{G},3}=0\ ; \tag{2}$$

when the electric field is in the plane of propagation perpendicular to the rods (p polarization), Maxwell's equations become

$$\sum_{\mathbf{G}'}(\mathbf{k}+\mathbf{G})\cdot(\mathbf{k}+\mathbf{G}-\mathbf{G}')d_{\mathbf{G}'}A'_{\mathbf{G}-\mathbf{G}'}-\omega^2 A'_{\mathbf{G}}=0\ , \tag{3}$$

where $A'_{\mathbf{G}}=A_{\mathbf{G},1}-A_{\mathbf{G},2}$. The coefficients $d_{\mathbf{G}'}$ are the Fourier-expansion coefficients of the inverse square of the position-dependent refraction index. The wave frequency is normalized with respect to the length of a unit cell of the lattice. The dispersion curves for s and p polarizations can be found from Eqs. (2) and (3), respectively. We have solved these equations using standard matrix diagonalization methods. The results that follow were tested with matrices of dimensions 441×441 and 841×841. The gap widths were estimated to be accurate to within 1%.

We first investigate arrays of air holes in a dielectric material. Figure 1 shows the dispersion relations for a square lattice of air rods with a filling fraction of 67% in a dielectric material of index 4.25. The cross section of the rods is square in (a) and circular in (b). The lower s bands are very similar in both structures, except for a degeneracy at the Γ symmetry point in the structure with circular rods; both structures yield an s gap across all symmetry points between the first and second bands and third and fourth bands, the larger s gap occurring in the array of circular rods. In the case of the lower p bands, there is a significant difference in the two structures; the array of square rods yields a p gap between the first and second bands while the array of circular rods yields a p

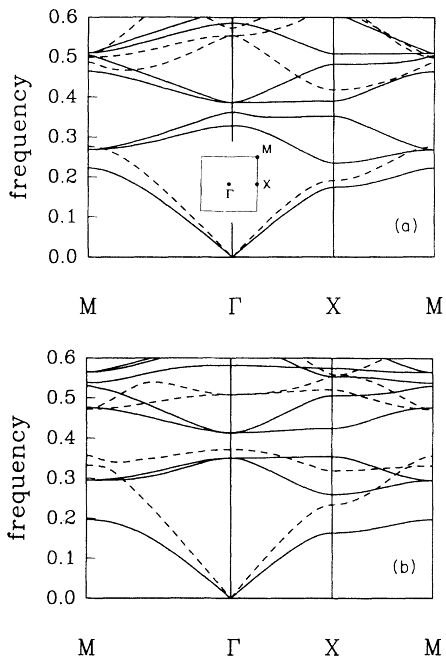

FIG. 1. Photonic band structure of a square lattice of air rods with a filling fraction of 67% in a dielectric material of index 4.25 for s (——) and p (– – –) polarizations. The cross section of the rods is square in (a) and circular in (b). The frequency is given in units of $2\pi c/a$, where a is the length of a unit cell. The inset shows the first Brillouin zone.

gap between the second and third bands (and can also yield a gap between the first and second bands for another set of parameters). The larger p gap occurs in the array of square rods. The aforementioned observations will play an important role in finding the conditions to generate a band gap since the overlap of s and p gaps will not occur between the same bands in arrays of square rods and circular rods.

Although both structures can give rise to an s gap between the first and second bands, we have not been able to generate an overlap between the lower s gap and a p gap. Figure 1 shows, however, that there is an overlap of the second s gap and first p gap in both structures. These s and p gaps overlap completely in the array of square rods and only partially in the array of circular rods. The gap width to midgap frequency ratio is 6.5% in the array of square rods and 10.4% in the array of circular rods. By changing the index contrast and/or the filling fraction, the s and p gaps can be made to shift and change in size. The overlap of s and p gaps is shown in Fig. 2 as a function of the filling fraction for an index contrast of 4.25. The overlap is normalized with respect to the midgap frequency.

For such an index contrast, the array of circular rods yields a larger gap than the array of square rods, when the filling fraction is 67% (as was shown in Fig. 1). The largest gap is 10.7% in an array of square rods (when the filling fraction is 75%) and 11% in an array of circular rods (when the filling fraction is 68%). Complete gaps exist for a wider range of filling fractions when the cross section of the rods is square. Although s and p gaps exist

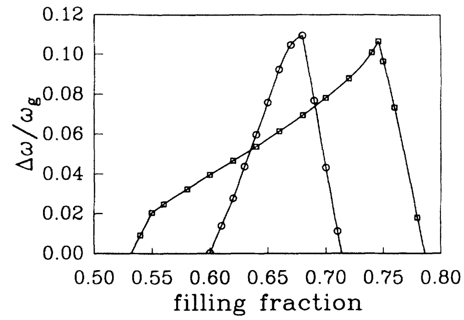

FIG. 2. Ratio of the gap width ($\Delta\omega$) to the midgap frequency (ω_g) as a function of the filling fraction of the air rods in a square lattice of index 4.25. The circles correspond to rods with circular cross section and the squares correspond to rods with square cross section.

outside this range of filling fractions, there is no overlap. The discontinuities in Fig. 2 indicate a change of the upper and lower bands limiting the gap width in going, for example, from partial to complete overlap of s and p gaps.

The largest band gap generated in a square lattice is shown in Fig. 3 as a function of the index contrast. The largest gap is taken over all filling fractions; thus, each point corresponds to a different filling fraction. An array of circular rods requires a significantly lower index contrast to generate a band gap than an array of square rods. Indeed, the minimum index contrast required for the s and p gaps to overlap is 2.70 in an array of circular rods and 3.51 in an array of square rods. It is known[6,7] that hexagonal lattices of rods with circular cross section require a minimum index contrast of 2.66 to generate a band gap. Since the hexagonal lattice has a more circle-like Brillouin zone than the square lattice, the gaps should be more likely to overlap across all symmetry points. However, the similarity between the minimum index contrast required to generate a gap in either square or hexagonal lattices with circular rods seems to suggest that the shape of the lattice is not the dominant parameter in trying to open a gap common to s and p polarizations in a two-dimensionally periodic structure, since s

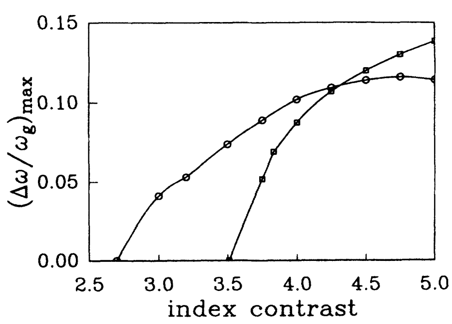

FIG. 3. Maximum gap width to midgap frequency ratio in a square lattice as a function of the index contrast. The circles correspond to rods with circular cross section and the squares correspond to rods with square cross section. The filling fraction of the rods is different for each point of the curves.

and p bands are not degenerate at the symmetry points. Rather, it is the shape of the rods that seems to play an important role in determining the conditions to open a gap in a square lattice. It has been shown,[6] however, that hexagonal lattices can give rise to significantly larger gaps than square lattices.

Although an array of circular rods requires a lower index contrast to generate a band gap than an array of square rods, Fig. 3 shows that the latter gives rise to a larger band gap when the index contrast is greater than 4.3. For example, when the index contrast is 5, the largest gap is 13.8% in an array of square rods and 11.4% in an array of circular rods. Furthermore, there seems to exist a maximum gap width that can be generated in an array of circular rods. The small drop of the gap width at index 5.0 with respect to the value at 4.75 is probably due to an increasing numerical error of the gap width as the index contrast increases.

We have also examined the band structure of dielectric rods in air. Such arrays of either square or circular rods can give rise to band gaps for s and p polarizations, but we have not been able to find any condition under which the s and p gaps overlap.

In summary, we have shown that periodic arrays of low-index rods with either a square or circular cross section located on a square lattice in a dielectric background of higher index exhibit photonic band gaps common to s and p polarizations. Arrays of rods with a circular cross section require a lower index contrast (2.70) to generate a band gap than rods with a square cross section (3.51). Furthermore, when the index contrast is greater than 4.3, arrays of square rods can give rise to larger gaps than arrays of circular rods.

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