Complete photonic band gap in a two-dimensional chessboard lattice

Mario Agio and Lucio Claudio Andreani
INFM—Dipartimento di Fisica ''A. Volta,'' Università di Pavia, via Bassi 6, I-27100 Pavia, Italy
(Received 14 October 1999; revised manuscript received 27 January 2000)

The photonic structure of a two-dimensional square lattice with square columns rotated by 45° is theoretically studied. For a range of dielectric filling factors around $f=0.5$ (for which the lattice reduces to a chessboard) a photonic band gap common to *s* and *p* polarizations is found. The complete band gap occurs for a wide range of values of the dielectric contrast and is maximum for relatively low values of the contrast.

Photonic crystals have attracted much interest in recent years, after the pioneering suggestions[1,2] that a photonic band gap (PBG) could lead to inhibited spontaneous emission and light localization. Much attention has been devoted to the problem of finding three-dimensional structures that forbid propagation of light in all directions, see e.g., Refs. 3–5. Two-dimensional (2D) photonic crystals have also been intensively studied,[6–18] since they are easier to fabricate (particularly in the optical region) and may be employed in waveguide configurations.[15,16] An important problem in this context is to find structures that, for light propagating in the plane, support a PBG common to polarizations of the electric field perpendicular (*s*) and parallel (*p*) to the plane.

A complete PBG in two dimensions was first demonstrated for a triangular lattice of air columns in a dielectric material[7,8] and for a square lattice of air columns.[8,9] It was later demonstrated for the hexagonal lattice with the graphite and BN structures.[13] For a given type of lattice symmetry, the PBG depends on the form of the basis and on the dielectric contrast.[19] For the triangular lattice a full PBG exists in the case of air columns (not for dielectric columns), and is maximum for a circular cross section of the columns.[8,10] Similarly, for the square lattice a complete PBG was shown only for the case of air columns; it exists for a circular or a square cross section of the columns, but in the latter case it requires a higher dielectric contrast.[9] The width of the gap of the square lattice may be increased by a suitable basis.[14] Physical arguments suggest that a PBG for *s* polarization is favored in the case of dielectric columns, while a PBG for *p* polarization is favored if the dielectric regions are connected.[3,7] However the existence of a complete PBG requires *overlap* of the *s* and *p* gaps: since this overlap often involves the gap between the first and second *p* bands with the gap between higher *s* bands, it is difficult to give simple arguments predicting (or explaining) the existence of a complete PBG for a given lattice.

In this work we study a different type of square photonic lattice in two dimensions, which consists of square columns of either dielectric or air rotated by 45° with respect to the square axes of the lattice (see Fig. 1). The structure is characterized by the filling factor *f* of the dielectric, which is related to the lattice constant *a* and the column diagonal *b* by $f=b^2/(2a^2)$ [in the case of dielectric columns, Fig. 1(a)] or $f=1-b^2/(2a^2)$ [for air columns, Fig. 1(b)]. For the close-packed condition $b=a$, or $f=0.5$, the two cases of Figs. 1(a) and 1(b) become equivalent and the structure resembles a chessboard. We shall refer to the structure of Fig. 1 as a ''chessboard'' lattice for every value of *f*. We find that a complete PBG exists in a range of filling factors around $f=0.5$ and is maximum for the case of dielectric columns. This is at variance with the ''conventional'' square lattice with square columns.[9] Furthermore, the complete PBG exists in a wide range of dielectric constrasts and is maximum for a relatively low value of ϵ, that is $\epsilon \simeq 8.9$. This makes the present square lattice an interesting candidate for experimental studies.

Photonic band structures are obtained solving Maxwell equations in macroscopic media with a periodic dielectric constant $\epsilon(\mathbf{r})$. Assuming nonmagnetic and lossless media [$\mu \simeq 1, \epsilon(\mathbf{r})$ real], absence of free currents and charges, we rearrange Maxwell equations in a master equation for the electric field $\mathbf{E}$:

$$\nabla \times \nabla \times \mathbf{E} = \frac{\omega^2}{c^2}\epsilon(\mathbf{r})\mathbf{E}, \tag{1}$$

plus the divergence equation $\nabla \cdot \epsilon(\mathbf{r})\mathbf{E}=0$, where ω is the frequency of harmonic modes. For a 2D photonic crystal, the dielectric constant is periodic in the $(\hat{\mathbf{x}},\hat{\mathbf{y}})$ plane and homogeneous along the $\hat{\mathbf{z}}$ direction: $\epsilon=\epsilon(x,y)$. Considering in-plane propagation, $k_z=0$, mirror symmetry decouples the electromagnetic field into two modes: *s* polarization (E_z, H_x, H_y) and *p* polarization (E_x, E_y, H_z). Since $\epsilon(\mathbf{r})$ is periodic, we exploit Bloch's theorem expanding the electro-

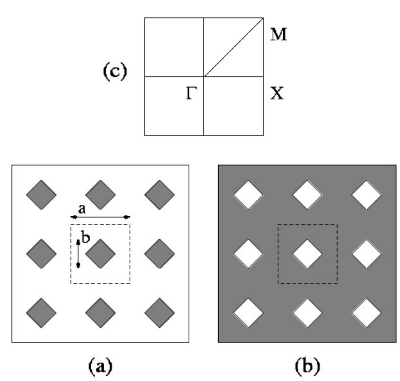

FIG. 1. The chessboard lattice: (a) dielectric rods in air, (b) air rods in dielectric. The dashed line marks the unit cell, *a* is the length of the unit cell and *b* is the rod's diagonal; (c) the Brillouin zone with symmetry points, Γ, X, M.

magnetic field in terms of plane waves. Different plane waves are coupled by the Fourier transform of the dielectric constant ϵ_{G_x,G_y}, which for our structure takes the form

$$\epsilon_{0,0}=\epsilon f+(1-f), \quad \mathbf{G}=\mathbf{0}$$

$$\epsilon_{G_x,G_y}=4(\epsilon-1)\frac{\cos(G_y b/2)-\cos(G_x b/2)}{a^2(G_x^2-G_y^2)},$$

$$\epsilon_{G_x,\pm G_x}=(\epsilon-1)b\frac{\sin(G_x b/2)}{a^2 G_x}, \quad \mathbf{G}\neq\mathbf{0} \tag{2}$$

where **G** is a reciprocal lattice vector and G_x and G_y are its components along $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$, respectively. The resulting **k**-space equations are solved by a matrix diagonalization technique. Photonic bands are calculated to about 1% precision including $\simeq 225$ plane waves for *s* modes and up to $\simeq 880$ plane waves for *p* modes. For the conventional square lattice, we recover results identical to those of Refs. 7 and 8, within the precision stated.

We present numerical results for the chess-board lattice of Fig. 1, for three choices of the dielectric contrast:[19] $\epsilon=8.9$ (alumina), $\epsilon=12$ (GaAs), and $\epsilon=16$ (Ge). An important feature of the chessboard lattice is that the structure with overlapping dielectric columns ($b>a$, $f>0.5$) is identical to a structure with nonoverlapping air columns ($b<a$ and the same filling fraction of dielectric). All configurations are spanned taking only nonoverlapping dielectric rods [$f<0.5$, Fig. 1(a)] or air rods [$f>0.5$, Fig. 1(b)]. The case $f=0.5$ identifies the close-packing condition for both dielectric and air rods, and makes the lattice invariant under the exchange dielectric $\leftrightarrow$ air.

Choosing alumina ceramic as dielectric medium ($\epsilon=8.9$), we find that photonic bands exhibit a complete PBG which is maximum for $f=0.45$, corresponding to a gap width to midgap frequency ratio $\Delta\omega/\omega=8.5\%$. For these parameters, the frequencies calculated along symmetry directions of the Brillouin zone are plotted in Fig. 2(a). The degeneracies at the symmetry points are the same of the conventional square lattice,[8,9] since the symmetry is the same: nondegenerate and doubly degenerate states at Γ and *M*, nondegenerate states at *X*. However the order of the frequency levels is different. There are three *s* gaps and just one *p* gap, which overlaps the second *s* gap giving rise to a complete PBG. Increasing the dielectric contrast, more *p* gaps open. With germanium ($\epsilon=16$), we find two complete PBG's: for $f=0.475$ the first PBG reaches its maximum width, $\Delta\omega/\omega=5.6\%$. Figure 2(b) shows the band structure calculated for $\epsilon=16$ and $f=0.475$. The higher dielectric contrast produces four *p* gaps and three *s* gaps. The second *s* gap overlaps again the first *p* gap; moreover, the third *s* gap overlaps the second *p* gap: thus two complete PBG's occur. These results are interesting considering that the traditional square lattice of air columns with square cross section requires $\epsilon>12.3$ for a complete PBG to exist. On the other hand, the chessboard lattice exhibits a complete PBG even for $\epsilon=8.9$ and preserves the symmetry and simplicity of the square lattice. Actually, spanning ϵ from 1 to 16, we find the existence of a complete PBG for $\epsilon>7$, with $\Delta\omega/\omega$ being maximum for ϵ close to 8.9.

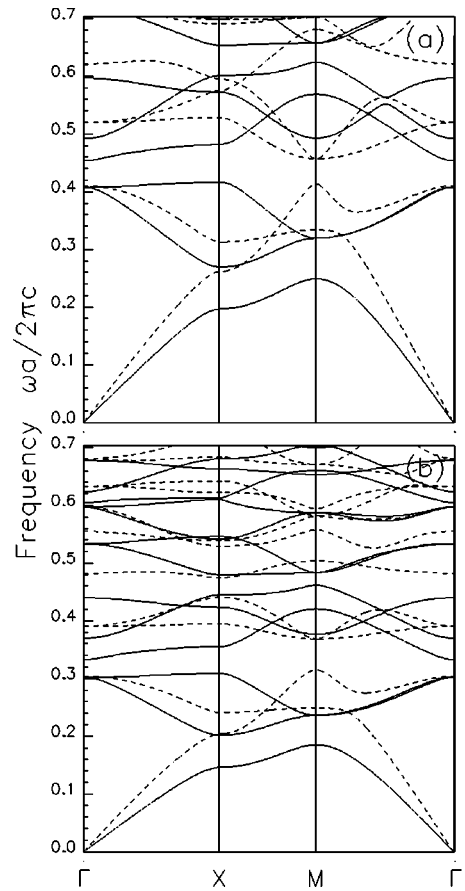

FIG. 2. Photonic bands of the chessboard lattice for (a) $\epsilon=8.9$, $f=0.45$ and (b) $\epsilon=16$, $f=0.475$ calculated along symmetry directions of the Brillouin zone. Solid (dashed) lines correspond to *s* (*p*) modes. Frequencies are plotted using the adimensional quantity $\omega a/(2\pi c)$, where *a* is the length of the unit cell and *c* the speed of light.

Figure 3 gives gap maps calculated for three different dielectric constants: $\epsilon=8.9,12,16$. Since the purpose is to find PBG's and to understand their behavior when the filling factor is varied, to save computing time, we used a maximum of $\simeq 570$ plane waves for *p* modes. Comparison with the photonic bands of Fig. 2 for the proper values of ϵ and *f* shows that numerical accuracy remains good. Fixing the dielectric contrast, the filling factor is varied from 0 to 1 and the existence of a PBG is marked with different tones to distinguish among only *s* (white), only *p* (gray), and complete PBG's (black). Generally, *s* gaps are concentrated in the left part of the plots, where $f<0.5$, that is the lattice is made up of dielectric rods in air: this agrees with the physical arguments discussed in Refs. 3 and 7. These PBG's fade away just when *f* becomes larger than 0.5 and the dielectric rods begin to overlap. Instead *p* gaps occur around the value $f=0.5$ and are the only existing gaps for $f>0.5$, when the dielectric regions are connected.[3,7] Thus, close to $f=0.5$, the chessboard lattice exhibits *s* gaps as well as *p* gaps, since at the close-packing condition the lattice possesses both dielectric columns and connectivity.

On increasing the filling factor the midgap frequency lowers. The same happens when ϵ increases from 8.9 to 16. Therefore, the midgap frequency should be related to the effective dielectric constant ϵ_{eff}, which is derived in the

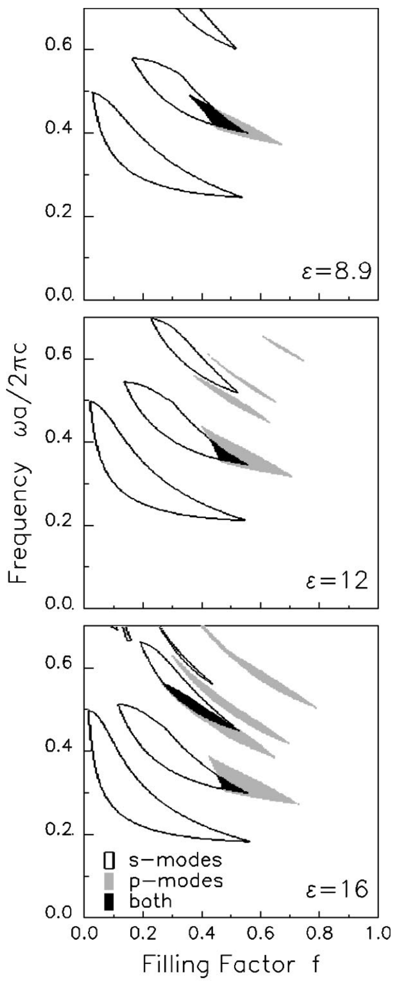

FIG. 3. Gap maps for different dielectric contrasts obtained varying the filling factor from 0 to 1. The existence of a PBG for both polarizations is represented by a black spot.

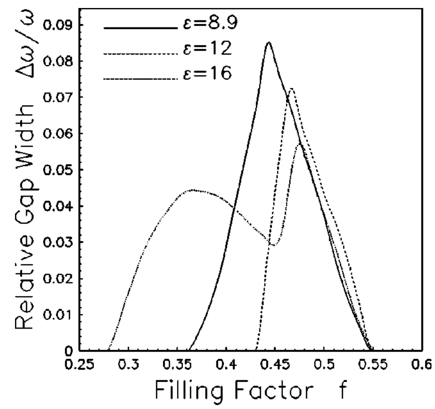

FIG. 4. Gap width to midgap frequency ratio plotted with respect to the filling factor for three dielectric contrasts: solid line for $\epsilon=8.9$, dashed line for $\epsilon=12$ and dotted line for $\epsilon=16$ (in this case only the largest $\Delta\omega/\omega$ is represented for each value of f).

long-wavelength limit. Moreover, a larger dielectric contrast widens PBG's and gives origin to additional ones, as shown in Fig. 3. For $\epsilon=8.9$ the second *s* gap overlaps the first (and unique) *p* gap. One would expect this complete PBG to get larger as the dielectric contrast is increased. On the contrary, the gap shrinks because *s* and *p* gaps have a smaller overlap. In fact, since *s* and *p* modes are decoupled and are governed by different equations, the overlap does not follow a simple rule and can be optimized for a right choice of f and ϵ. However, a larger dielectric contrast provides more PBG's, making complete PBG's more likely to occur. This is what happens for $\epsilon=16$: a new complete PBG comes from the overlap of the third *s* gap and the second *p* gap. In this case, the chessboard lattice exhibits two complete PBG's, the first one maximizes its width for $f=0.475$ and the second one for $f\simeq 0.38$. Besides, the second PBG occurs at a higher frequency and for a wider range of the filling factor than the first one.

In Fig. 4 the gap width to midgap frequency ratio is plotted with respect to the filling factor for the complete PBG's shown in Fig. 3. The maximum fractional gap is for $\epsilon=8.9$. When the dielectric contrast is raised, the peak corresponding to the lowest complete PBG lowers and shrinks; it also becomes restricted to a narrow region around the close-packing condition $f=0.5$. The smooth peak of the dotted curve ($\epsilon=16$) is due to the second complete PBG, which extends for a wider range of filling fractors. The first and second complete PBG's for $\epsilon=16$ are of comparable width $\Delta\omega$, but the fractional gap is obviously smaller for the second one.

The chessboard lattice is found to have a complete PBG arising from overlap of the second *s* gap with the first *p* gap. The full PBG exists for a range of filling factors around the close-packing condition $f=0.5$, provided the dielectric constant $\epsilon>7$, and it reaches a maximum for $\epsilon\sim 8.9$ and $f=0.45$ with a fractional gap $\Delta\omega/\omega=8.5\%$. On increasing the dielectric contrast the complete PBG decreases somewhat. For $\epsilon=16$ a second complete PBG arises from overlap of the third *s* gap with the second *p* gap, and is maximum for $f=0.38$.

The gap maps as a function of filling factor show that *s* gaps are favored for the case of nonoverlapping dielectric columns ($f<0.5$), while *p* gaps are favored in the case of air columns ($f>0.5$). Although the overlap of *s* and *p* gaps does not follow a simple rule, the existence of a complete PBG is related to the fact that the chessboard lattice, at the close-packing condition ($f=0.5$), has both dielectric columns and connected dielectric regions. The chessboard lattice has the same symmetry and simplicity of the conventional square lattice: the low dielectric contrast required for the existence of a complete gap makes it interesting for experimental studies.

Note added. Recently a paper by Wang *et al.*, has been published,[20] where the square lattice with rotated square columns is also studied.

The authors are grateful to S. Botti, A. Lorenzoni, and A. Rappoldi for helpful suggestions and advice in the course of this work and to C. M. Soukoulis for a critical reading of the manuscript.

[1] E. Yablonovitch, Phys. Rev. Lett. **58**, 2059 (1987).
[2] S. John, Phys. Rev. Lett. **58**, 2486 (1987).
[3] J. D. Joannopoulos, R. D. Meade, and J. N. Winn, *Photonic Crystals—Molding the Flow of Light* (Princeton University Press, Princeton, NJ, 1995).
[4] *Photonic Band Gaps Materials*, Vol. 315 of *NATO Advanced Studies Institute, Series E: Applied Sciences*, edited by C. M. Soukoulis (Kluwer, Dordrecht, 1996).
[5] *Microcavities and Photonic Band Gaps: Physics and Applications*, Vol. 324 of *NATO Advanced Studies Institute, Series E: Applied Sciences*, edited by C. Weisbuch and J. Rarity (Kluwer, Dordrecht, 1996).
[6] W. M. Robertson *et al.*, Phys. Rev. Lett. **68**, 2023 (1992); J. Opt. Soc. Am. B **10**, 322 (1993).
[7] R. D. Meade, K. D. Brommer, A. M. Rappe, and J. D. Joannopoulos, Appl. Phys. Lett. **61**, 495 (1992); J. Opt. Soc. Am. B **10**, 328 (1993).
[8] P. R. Villeneuve and M. Piché, Phys. Rev. B **46**, 4969 (1992).
[9] P. R. Villeneuve and M. Piché, Phys. Rev. B **46**, 4973 (1992).
[10] R. Padjen, J.-M. Gérard, and J.-Y. Marzin, J. Mod. Opt. **41**, 295 (1994).
[11] P. L. Gourley *et al.*, Appl. Phys. Lett. **64**, 687 (1994).
[12] T. Baba and T. Matsuzaki, Jpn. J. Appl. Phys. **34**, 4496 (1995).
[13] D. Cassagne, L. Jouanin, and D. Bertho, Phys. Rev. B **52**, 2217 (1995); **53**, 7134 (1996).
[14] C. M. Anderson and K. P. Giapis, Phys. Rev. Lett. **77**, 2949 (1996); Phys. Rev. B **56**, 7313 (1997).
[15] T. F. Krauss, R. M. De La Rue, and S. Brand, Nature (London) **383**, 699 (1996).
[16] D. Labilloy *et al.*, Phys. Rev. Lett. **79**, 4147 (1997).
[17] J. D. Joannopoulos, P. R. Villeneuve, and S. Fan, Nature (London) **386**, 143 (1997).
[18] Z.-Y. Li, B.-Y. Gu, and G.-Z. Yang, Phys. Rev. Lett. **81**, 2574 (1998).
[19] The photonic structure (apart from a scale factor) depends only on the ratio $\epsilon_2:\epsilon_1$ of the dielectric constants of the constituents. Following common practice, we take the material with lower dielectric constant to be air, and set $\epsilon_1=1$, $\epsilon_2=\epsilon$.
[20] X.-H. Wang, B.-Y. Gu, Z.-Y. Li, and G.-Z. Yang, Phys. Rev. B **60**, 11 417 (1999).