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# Symmetry, degeneracy, and uncoupled modes in two-dimensional photonic lattices

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The photonic bands of two-dimensional triangular and square lattices composed of circular rods were classified by means of the group theory based on the symmetry of the lattice structure. According to this classification, it was shown that the uncoupled mode, or the mode that cannot be excited by an external plane wave, which we previously found for the triangular lattice by the numerical calculation of the transmittance, is an antisymmetric mode under the relevant mirror reflection, and this fact is consistent with the observation by Robertson *et al.* It was also shown that triangular and square lattices with $C_{6v}$ or $C_{4v}$ symmetry have many other uncoupled modes with relatively low eigenfrequencies and some of them can be easily identified as the spectral ranges of total reflection in spite of their nonzero state density.

Periodic dielectric structures, which are called photonic crystals or photonic lattices, have attracted much interests in recent years.[1–17] The main reason for the intensive investigations is that a photonic band gap, in which the existence of any electromagnetic modes is forbidden, can be realized by the proper design of the lattice structure.[3,5,16] Many peculiar physical phenomena due to the photonic band gap, such as the suppression of spontaneous emission[1] and energy transfer,[7] and localized donor and acceptor modes,[2,11] have been predicted and some of them were confirmed experimentally. Beside the emergence of the photonic band gap, the enhanced state density and the extraordinary low group velocity at the band edges are expected to bring about many new possibilities in optical physics.

The band structure of the photonic lattices has been investigated by observing the transmission spectra of the specimens. The observed opaque spectral ranges were successfully compared with the band gaps obtained by the band calculation performed for the corresponding infinite lattices, for which the Bloch's theorem is applicable to the relevant electromagnetic wave equation and the computational task is much reduced.[3,8] Although this kind of comparison is correct concerned with the band gaps, it neglects the effect of the coupling strength between the incident/transmitted wave and the internal electromagnetic field at the surface of the specimen, the energy transfer to Bragg waves, and the interference between the front and the rear surfaces of the specimen.

In fact, our recent calculation of the transmission spectra of a two-dimensional (2D) triangular photonic lattice showed that the modification of the spectra by these three features is quite pronounced.[17] Especially, we found the existence of an uncoupled mode, which cannot be excited by an external plane wave. This fact was confirmed experimentally for a 2D air-rod lattice formed in a block of methylpentene polymer in the far-infrared region.[18] Our method is based on the Fourier expansion of the internal field and fully allows for the boundary condition at the surface of the specimen, and is applicable to any kind of 2D photonic lattices as long as the wave vector of the incident field lies in the 2D plane. The existence of uncoupled modes was first discussed by Robertson *et al.*[9] They compared the dispersion relation of a 2D square lattice observed by their coherent microwave transient spectroscopy technique with that by the band calculation, and found that the antisymmetric modes under the mirror reflection at the plane, which includes the incident wave vector and is perpendicular to the 2D plane, were not observed in their experiment. They argued that the incident plane wave does not excite these antisymmetric modes because the former is symmetric under the same mirror reflection, and hence, the effective coupling between them is zero.

In this paper, we will show by means of a group theoretical classification of the photonic bands based on the symmetry of the lattice structure that the uncoupled mode in the 2D triangular lattice, which we found by the numerical calculation of the transmission spectra in the previous paper,[17] really belongs to the category discussed by Robertson *et al.* We will also show that 2D triangular and square lattices with $C_{6v}$ or $C_{4v}$ symmetry have many other uncoupled modes and some of them can be easily identified as spectral ranges of total reflection in spite of their nonzero state density.

Now, the vector wave equations derived from Maxwell's equations can be reduced to two independent scaler equations when the wave vector lies in the 2D plane,[11–13] or in other words, the fields are independent of the $z$ coordinate. (The $z$ axis is taken as perpendicular to the 2D plane.) These two modes are called $H$ polarization, for which the magnetic field is parallel to the $z$ axis, and $E$ polarization, for which the electric field is parallel to the $z$ axis, respectively. The magnetic field for $H$ polarization ($H_z$) satisfies the next equation:[13]

$$\mathcal{L}_H H_z \equiv -\left[\frac{\partial}{\partial x}\frac{1}{\epsilon(\mathbf{x}_\parallel)}\frac{\partial}{\partial x}+\frac{\partial}{\partial y}\frac{1}{\epsilon(\mathbf{x}_\parallel)}\frac{\partial}{\partial y}\right]H_z=\frac{\omega^2}{c^2}H_z, \tag{1}$$

 

whereas the electric field for $E$ polarization ($E_z$) is governed by the following equation:[13]

$$\mathcal{L}_E E_z \equiv -\frac{1}{\epsilon(\mathbf{x}_\parallel)}\left[\frac{\partial^2}{\partial^2 x}+\frac{\partial^2}{\partial^2 y}\right]E_z=\frac{\omega^2}{c^2}E_z. \qquad (2)$$

In Eqs. (1) and (2), $\mathbf{x}_\parallel$ is the 2D position vector $(x,y)$, $\epsilon(\mathbf{x}_\parallel)$ is the position-dependent dielectric constant, $c$ is the light velocity in vacuum, and $\omega$ is the eigenangular frequency.

Next, we consider the symmetry of the 2D triangular and square lattice composed of circular rods. The position-dependent dielectric constant is invariant under a symmetry operation, which belongs to $C_{6v}$ point group for the triangular lattice or $C_{4v}$ point group for the square lattice. Namely, if we denote the symmetry operation by $R$,

$$R\epsilon(\mathbf{x}_\parallel)R^{-1}=\epsilon(\overleftrightarrow{R}^{-1}\mathbf{x}_\parallel)=\epsilon(\mathbf{x}_\parallel), \qquad (3)$$

where $\overleftrightarrow{R}$ denotes the $2\times 2$ matrix representation of the symmetry operation $R$. Because $R$ is a rotation or a mirror reflection operator, $\overleftrightarrow{R}$ is an orthogonal matrix, i.e.,

$$\overleftrightarrow{R}^t\overleftrightarrow{R}=\overleftrightarrow{E}, \qquad (4)$$

where $\overleftrightarrow{R}^t$ is the transposed matrix of $\overleftrightarrow{R}$ and $\overleftrightarrow{E}$ is the unit matrix. Using these two relations, we can prove that $R$ commutes with $\mathcal{L}_H$ and $\mathcal{L}_E$:

$$R\mathcal{L}_H R^{-1}=\mathcal{L}_H, \qquad R\mathcal{L}_E R^{-1}=\mathcal{L}_E. \qquad (5)$$

Therefore, any eigenfunction of $\mathcal{L}_H$ or $\mathcal{L}_E$ is an eigenfunction of $R$ as well. So, the conventional classification of eigenmodes based on the group theory, which is familiar to the electronic band theory, is applicable to the present problem.[19]

The 2D Brillouin zone of the triangular lattice possesses two highly symmetric points beside the $\Gamma$ point at the center of the zone: the $J$ point whose wave vector is $\pi/a(4/3,0)$ and the $X$ point whose wave vector is $\pi/a(1,1/\sqrt{3})$, where the elementary lattice vectors are denoted by $(a,0)$ and $(a/2,\sqrt{3}a/2)$. Table I shows the symmetry of these points and the irreducible representaions for several low eigenfrequencies. The eigenfrequencies, which are expressed in a dimensionless form by the use of the lattice constant $a$ and the light velocity $c$, were calculated for plane waves in vacuum whose wave vectors were reduced to the first Brillouin zone of the triangular lattice. Because the dielectric constant of the material that we concider in this paper is not very large, and hence, the dispersion relation is not very far from that in vaccum, we can assign a corresponding irreducible representation to each band of the actual lattice by consulting this table. Table II shows the compatibility relation between the irreducible representations for the above three points and those for the wave vector on segment $\overline{\Gamma J}$ and segment $\overline{\Gamma X}$. Only one mirror reflection is defined on these segments because of their low symmetry. In Table II, the wave function ($H_z$ or $E_z$) of mode $A$ on segment $\overline{\Gamma J}$ ($\overline{\Gamma X}$) is symmetric under the mirror reflection at the plane which includes the $z$ axis and segment $\overline{\Gamma J}$ ($\overline{\Gamma X}$), whereas that of mode $B$ is antisymmetric under the same mirror reflection. Therefore, mode $B$ is identified as an uncoupled mode according to Robertson *et al.*

TABLE I. The irreducible representations for the electromagnetic waves in vacuum, whose wave vectors are reduced in the first Brillouin zone of the triangular lattice.

| Wave vector | Symmetry | $\omega a/2\pi c$ | Representation |
|---|---|---|---|
| $\Gamma$ | $C_{6v}$ | 0 | $A_1$ |
| | | $2/\sqrt{3}$ | $A_1+B_2+E_1+E_2$ |
| | | 2 | $A_1+B_1+E_1+E_2$ |
| $J$ | $C_{3v}$ | 2/3 | $A_1+E$ |
| | | 4/3 | $A_1+E$ |
| | | $2\sqrt{7}/3$ | $A_1+A_2+2E$ |
| $X$ | $C_{2v}$ | $1/\sqrt{3}$ | $A_1+B_1$ |
| | | 1 | $A_1+B_2$ |
| | | $\sqrt{7/3}$ | $A_1+A_2+B_1+B_2$ |

Figures 1(a) and 1(b) show the dispersion relation of the triangular lattice for $H$ polarization and $E$ polarization, respectively. The dielectric constants of the circular rod and the background were assumed to be 1.0 (air) and 2.1 (methylpentene), respectively. The lattice constant $a$ was taken as 170 $\mu$m, and the radius of the rod was 62.5 $\mu$m. The dispersion relation was calculated by the plane-wave expansion method according to Plihal and Maradudin[13] with 271 basis plane waves, and the computational error was estimated as less than 1%. The mode assignment obtained from Tables I and II is also shown in Figs. 1(a) and 1(b), where notations such as $A_1(B_1)$ and $A_1+B_1$ mean that the assignment is not rigorously accomplished with the knowledge of the group theory alone. The band degeneracy at the highly symmetric points is consistent with the classification by the group theory. First, we find that the second lowest band along the $\Gamma$-$J$ direction for $E$ polarization, which was identified as an uncoupled mode in the previous paper,[17] is really mode $B$. Therefore, the wave function of this mode ($E_z$) is antisymmetric under the mirror reflection mentioned above, and this is the reason why it does not couple to

TABLE II. The compatibility relations in the triangular lattice.

| Representation at highly symmetric points | Representation on segment $\overline{\Gamma J}$ | Representation on segment $\overline{\Gamma X}$ |
|---|---|---|
| $\Gamma(A_1)$ | $A$ | $A$ |
| $\Gamma(A_2)$ | $B$ | $B$ |
| $\Gamma(B_1)$ | $A$ | $B$ |
| $\Gamma(B_2)$ | $B$ | $A$ |
| $\Gamma(E_1)$, $\Gamma(E_2)$ | $A+B$ | $A+B$ |
| $J(A_1)$ | $A$ | |
| $J(A_2)$ | $B$ | |
| $J(E)$ | $A+B$ | |
| $X(A_1)$, $X(B_1)$ | | $A$ |
| $X(A_2)$, $X(B_2)$ | | $B$ |

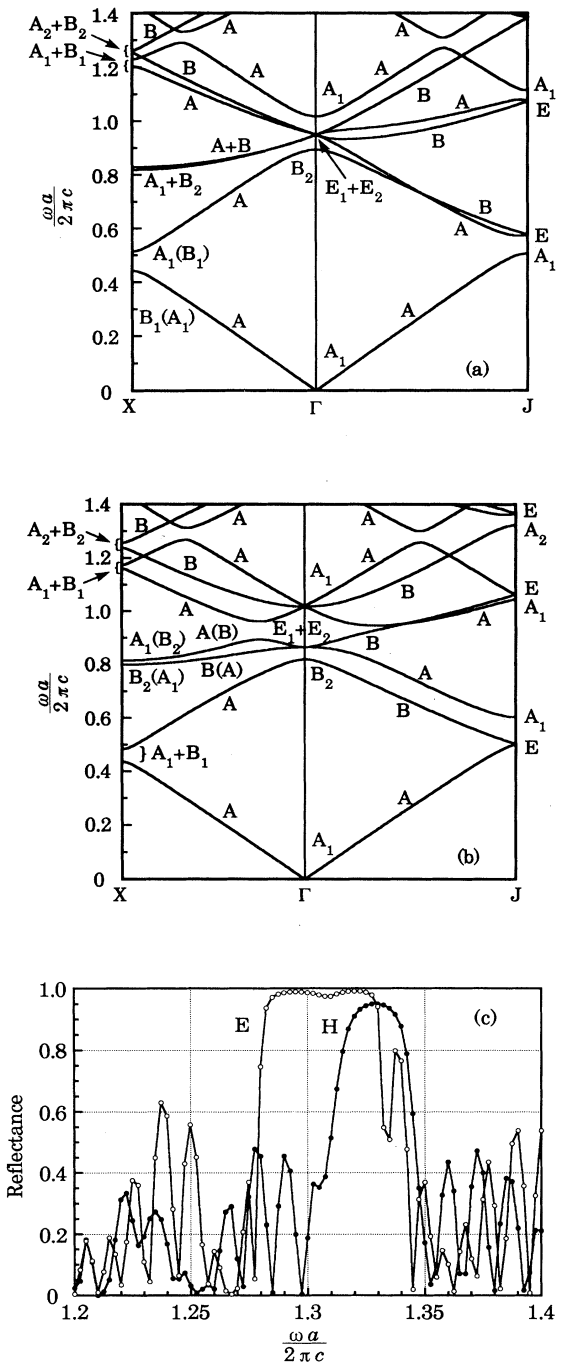





FIG. 1. The band structure and the reflection spectra of the 2D triangular lattice composed of circular rods. (a) The band structure for $H$ polarization, (b) the band structure for $E$ polarization, and (c) the reflection spectra along the $\Gamma$-$X$ direction for both polarizations. The following parameters were used: the lattice constant $a$ is 170 $\mu$m, the radius of the rod is 62.5 $\mu$m, and the dielectric constants of the rod and the background are 1.0 (air) and 2.1 (methylpentene), respectively. For the calculation of the reflectance, we further assumed that the distance between the surface and the first layer of the rods is 900 $\mu$m and the number of the layers is 22.

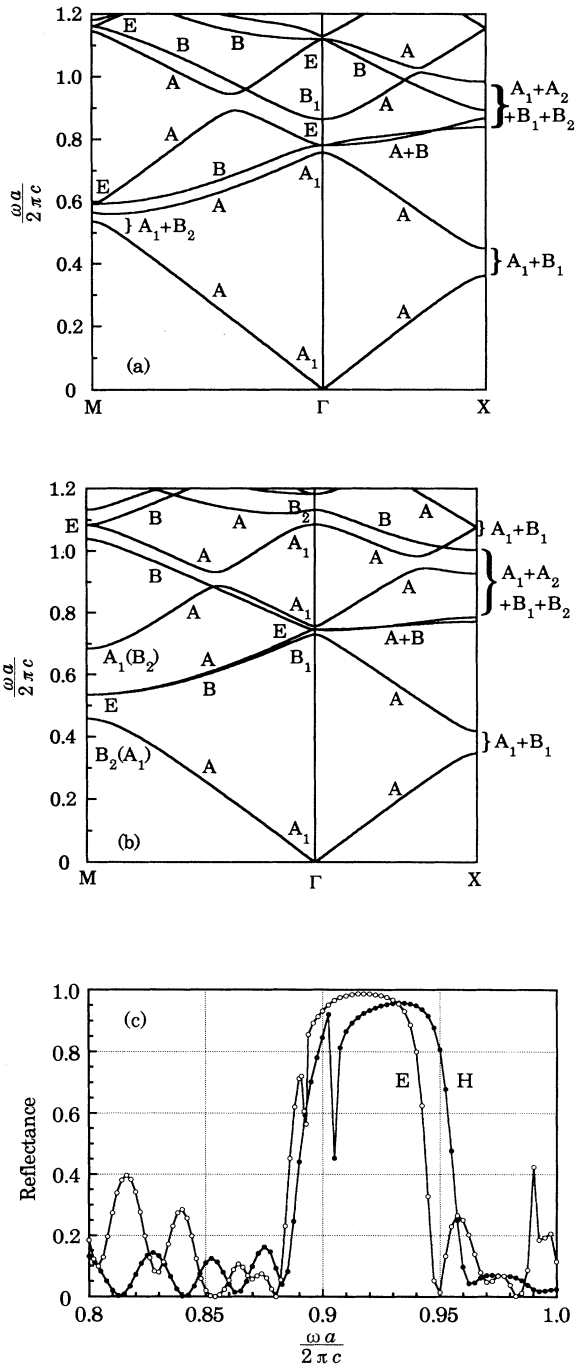





FIG. 2. The band structure and the reflection spectra of the 2D square lattice composed of circular rods. (a) The band structure for $H$ polarization, (b) the band structure for $E$ polarization, and (c) the reflection spectra along the $\Gamma$-$M$ direction for both polarizations. The following parameters were used: the lattice constant $a$ is 1.17 $\mu$m, the radius of the rod is 0.504 $\mu$m, and the dielectric constants of the rod and the background are 1.0 (air) and 2.72 (PbO glass), respectively. For the calculation of the reflectance, we further assumed that the distance between the surface and the first layer of the rods is 1.0 $\mu$m and the number of the layers is 14.

TABLE III. The irreducible representations for the electromagnetic waves in vacuum whose wave vectors are reduced in the first Brillouin zone of the square lattice.

| Wave vector | Symmetry | $\omega a/2\pi c$ | Representation |
|---|---|---|---|
| $\Gamma$ | $C_{4v}$ | 0 | $A_1$ |
| | | 1 | $A_1 + B_1 + E$ |
| | | $\sqrt{2}$ | $A_1 + B_2 + E$ |
| | | 2 | $A_1 + B_1 + E$ |
| $M$ | $C_{4v}$ | $1/\sqrt{2}$ | $A_1 + B_2 + E$ |
| | | $\sqrt{10}/2$ | $A_1 + A_2 + B_1 + B_2 + 2E$ |
| $X$ | $C_{2v}$ | 1/2 | $A_1 + B_1$ |
| | | $\sqrt{5}/2$ | $A_1 + A_2 + B_1 + B_2$ |
| | | 3/2 | $A_1 + B_1$ |
| | | $\sqrt{13}/2$ | $A_1 + A_2 + B_1 + B_2$ |

TABLE IV. The compatibility relations in the square lattice.

| Representation at highly symmetric points | Representation on segment $\overline{\Gamma M}$ | Representation on segment $\overline{\Gamma X}$ |
|---|---|---|
| $\Gamma(A_1)$ | $A$ | $A$ |
| $\Gamma(A_2)$ | $B$ | $B$ |
| $\Gamma(B_1)$ | $B$ | $A$ |
| $\Gamma(B_2)$ | $A$ | $B$ |
| $\Gamma(E)$ | $A + B$ | $A + B$ |
| $M(A_1)$, $M(B_2)$ | $A$ | |
| $M(A_2)$, $M(B_1)$ | $B$ | |
| $M(E)$ | $A + B$ | |
| $X(A_1)$, $X(B_1)$ | | $A$ |
| $X(A_2)$, $X(B_2)$ | | $B$ |

the external plane wave at normal incidence. Second, we also find that there are several other frequency ranges where only a $B$ mode exists. We expect a total reflection at these ranges in spite of their nonzero state density. As an example, Fig. 1(c) shows the reflection spectra along the $\Gamma$-$X$ direction from $\omega a/2\pi c = 1.2$ to 1.4. These spectra were calculated by the plane-wave expansion method presented in the previous paper[17] with 1870 basis plane waves. We assumed that the distance between the surface and the first layer of the circular rods of the specimen was 900 $\mu$m and the number of the layers was 22. Here, we find a range of high reflectance (more than 0.9) from $\omega a/2\pi c = 1.319$ to 1.338 for $H$ polarization and from 1.282 to 1.330 for $E$ polarization. The spectral range where only a $B$ mode exsists is from $\omega a/2\pi c = 1.291$ to 1.331 for $H$ polarization and from 1.268 to 1.321 for $E$ polarization. Therefore, the deviation is less than 2.2% and we can conclude that the correspondence between the spectral ranges of high reflectance and those where only a $B$ mode exists is good. The wavy patterns below and above the ranges of total reflection are caused by the interference between the front and the rear surfaces of the assumed specimen.

Next, we examine the case of the square lattice. There are two highly symmetric points beside the $\Gamma$ point in the 2D Brillouin zone of the square lattice: the $M$ point whose wave vector is $\pi/a(1,1)$ and the $X$ point whose wave vector is $\pi/a(1,0)$. Table III shows the symmetry of these points and the irreducible representaions for several low eigenfrequencies. The eigenfrequencies were calculated for plane waves in vacuum as before. Their wave vectors were reduced to the first Brillouin zone of the square lattice in this case. Table IV shows the compatibility relation between the irreducible representations for the above three points and those for the wave vector on segment $\overline{\Gamma M}$ and segment $\overline{\Gamma X}$. The notation of mode $A$ and $B$ in Table IV is the same as before, i.e., the wave function of mode $A$ on segment $\overline{\Gamma M}$ ($\overline{\Gamma X}$) is symmetric under the mirror reflection at the plane which includes the $z$ axis and segment $\overline{\Gamma M}$ ($\overline{\Gamma X}$), whereas that of mode $B$ is antisymmetric under the same mirror reflection.

Figures 2(a) and 2(b) show the dispersion relation of the square lattice. In this case, the dielectric constants of the circular rod and the background were assumed to be 1.0 (air) and 2.72 (PbO glass), respectively. The lattice constant $a$ was taken as 1.17 $\mu$m, and the radius of the rod was 0.504 $\mu$m. The mode assignment obtained from Tables III and IV is also shown in Figs. 2(a) and 2(b). In these figures, we again find several frequency ranges where only a $B$ mode exists, for which we expect a total reflection as before. As an example, Fig. 2(c) shows the reflection spectra along the $\Gamma$-$M$ direction from $\omega a/2\pi c = 0.8$ to 1.0. Here, we find a range of high reflectance (more than 0.9) from $\omega a/2\pi c = 0.902$ to 0.947 for $H$ polarization and from 0.897 to 0.936 for $E$ polarization. The spectral range where only a $B$ mode exists is from $\omega a/2\pi c = 0.893$ to 0.945 for $H$ polarization and from 0.888 to 0.932 for $E$ polarization. Therefore, the correspondence between them is good again. (The deviation is less than 1.4%.)

In conclusion, we have classified the photonic bands of the 2D triangular and square lattices composed of circular rods according to the group theory based on the symmetry of the lattice structure. We have shown that the uncoupled mode in the triangular lattice, which we previously found by the numerical calculation of the transmittance, is an antisymmetric mode under the relevant mirror reflection. This fact is consistent with the observation by Robertson *et al.* We have also shown that 2D triangular and square lattices with $C_{6v}$ or $C_{4v}$ symmetry have many other uncoupled modes and some of them can be easily identified as the spectral ranges of total reflection in spite of their nonzero state density.

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