Irreducible Brillouin Zone for 2D Phononic Crystals with Different Configurations

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ABSTRACT

Plane-wave expansion method are employed to investigate the effect of point-group symmetry to the irreducible Brillouin zone (BZ) of two-dimensional phononic crystals (PCs). Based on the calculations of four kind configurations with different symmetry, we find that the irreducible BZ will enlarge with the lower of the point-group symmetry of PCs and some of the maximums or minimums of bands are not locate at the periphery of the irreducible BZ. Therefore, the previous calculations of band structure, considering only the periphery of the irreducible BZ, is incomplete for PCs with low point-group symmetry. We analyze this problem and give a guide for further investigations in the paper, which is important to obtain accurate band structure of PCs with low point-group symmetry.

INTRODUCTION

Significant efforts have been devoted to the study of phononic crystals (PCs) because of their novel physical properties and numerous potential applications, such as negative refraction, sonic focusing, elastic isolators, mirrors, filters and waveguides[1, 2, 3, 4, 5, 6]. Applications of PCs rely heavily on the existence of phononic band gaps (PBGs). Thus, various approaches have been used to search for structures that facilitate the formation of PBGs. The symmetry of PCs is one of the main factors in creating PBGs. Considering this concept, scientists have employed various methods to study the symmetry of the PCs. For instance, Zhong et al.[7] calculated five different shapes of steel rods (i.e., regular triangle, square, hexagon, octagon prisms and columns) that were placed in the air to form a square lattice crystal and discussed the dependency of the PBGs on the non-circular rod orientation and symmetry of rods. Chai et al.[8] studied the complete and directional PBGs properties of 2D mercury/air PCs with L-shape scatters, and their findings show that the PBGs widths could be widely adjusted by changing their geometry and rotating the L-shape scatters. S. Mohammadi et al.[9] found that PCs, preferably hexagonal

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lattice PCs with holes etched into a Si plate, have the ability to integrate PBGs functionalities using a CMOS-compatible fabrication process.

In general, we calculated PBGs along the periphery of the irreducible Brillouin zone (BZ). The symmetry of the PCs may consider the lattice and scatter symmetry. In previous studies, the scatterer and lattices of PCs were designed and the scatterer orientation and configuration were changed. Thus, the irreducible BZ and calculation may also be changed.

Dong et al. [10, 11] found that the bands of PCs are twisted in the entire area of the first BZ. This condition expands the irreducible BZ to the entire first BZ. The researchers investigated the effect of the basis configuration on the acoustic band structure in 2D complex PCs and found that the irreducible BZ of PCs might be changed when the basis configuration was changed. Hu et al. [12] found that it is necessary to study the whole first BZ to get rightly PBGs for elliptic rods because of some of the extrema of the acoustic bands located in specific lines.

However, the irreducible BZ does not need to expand to the entire first BZ for all structures of PCs. We further studied an additional atom in a unit cell and designed it in structures with different operation numbers of the point group symmetry. We also calculated the eigen-frequencies of the five lowest bands in the first BZ. Calculation results of the band structure of 2D PCs show that the irreducible BZ should be larger, whereas the PC point group symmetry should be lower.

THE MODEL AND METHOD

Figure 1. (a) 2D PCs model in a square lattice; (b) Unit cell with an additional rod; (c) 2D PCs with a square lattice.

We considered 2D PCs consisting of steel cylinders embedded in epoxy matrix in a square lattice as shown in Figure 1(a). The elastic parameters used in the calculations are \( \rho_s = 7890 \text{ Kg/m}^3 \), \( C_{st} = 5780 \text{ m/s}^{-1} \), and \( C_{et} = 3220 \text{ m/s}^{-1} \), for steel. \( \rho_s = 1100 \text{ Kg/m}^3 \), \( C_{st} = 2830 \text{ m/s}^{-1} \), and \( C_{et} = 1160 \text{ m/s}^{-1} \) for epoxy. To examine the band structures for PCs with different configurations, we considered that PCs have point groups, including different point group symmetry operations. The models are shown in Figures 2(a), 3(a), 4(a) and 5(a). The PCs with an additional rod in each unit cell are presented in Figure 1(b).

Figure 1(c) shows the first BZ for the square lattice. The basic triangle( ΓMX shaded area) is equivalent to the basic irreducible BZ. We defined other points (Figure 1c) to study the entire area of the first BZ.
We used the plane-wave expansion method to calculate the eigen-frequencies. This method has been used in numerous studies, and some provide the details of the calculated process[13, 14, 15, 16]. Approximately 625 plane waves were used to investigate the eigenvalue convergence in the current study. The convergence accuracy for the lowest acoustic bands is less than 1%. Typically, the reciprocal lattice points are used to diagonalize the matrices for the two-rod configuration in the unit cell.

THE RESULTS AND DISCUSSIONS

First, we placed an additional square rod at the centre of the unit cell (Figure 2a, $L_{1x} = L_{1y} = 0.30a$, $L_{2x} = L_{2y} = 0.30a$). The PCs with this configuration have $C_{4v}$ point group symmetry, including eight elements. The contours of the phononic band frequencies for the PCs with the unit cell shown in Figure 1(a) are displayed in the entire area of the first BZ for bands 1 (Figure 2b), 2 (Figure 2c), 3 (Figure 2d), 4 (Figure 2e) and 5 (Figure 2f). The triangle $\Gamma X$ shown by the solid line is the basic triangle (Figure 1c). The value of the band frequencies increases as the shade becomes darker. The dark and bright circles in the entire area of the first BZ indicate the minimum and maximum points, respectively. The same condition applies to Figures 3, 4 and 5. We examined the distributions carefully from bands 1 (Figure 2b) to 5 (Figure 2f). For bands 1 and 5, $\omega_{1}^\text{max}$ and $\omega_{5}^\text{max}$ occur at the centre point $\Gamma$, whereas $\omega_{1}^\text{min}$ and $\omega_{5}^\text{min}$ occurs at each unit corner, namely, M, M1, M2 and M3. For band 2, $\omega_{2}^\text{max}$ occurs at X, X1, Y and Y1, whereas $\omega_{2}^\text{min}$ is symmetrically distributed along the lines of $X\Gamma$, $X_{1}\Gamma$, $Y\Gamma$ and $Y_{1}\Gamma$. For band 3, $\omega_{3}^\text{max}$ occurs at the centre point $\Gamma$, whereas $\omega_{3}^\text{max}$ is symmetrically distributed along the lines of $M\Gamma$, $M_{1}\Gamma$, $M_{2}\Gamma$ and $M_{3}\Gamma$. For band $\omega_{4}^\text{max}$ occurs at X, X1, Y and Y1, whereas $\omega_{4}^\text{min}$ is symmetrically distributed along the lines of $M\Gamma$, $M_{1}\Gamma$, $M_{2}\Gamma$ and $M_{3}\Gamma$. All bands show a symmetric structure in the entire area of the first BZ. As a result of this symmetry, points that fall on the periphery of the basic triangle take the minimum and maximum frequency values for bands in the entire area of the first BZ. The irreducible BZ is one-eighth of the entire first BZ. Therefore, the band structures of PCs along the periphery of this region must be studied.
Figure 2. (a) 2D PC model with a square cylinder placed at the centre of the unit cell; (b-f) Contours of the five lowest eigen-frequencies in the first BZ for (b) band 1, (c) band 2, (d) band 3, (e) band 4 and (f) band 5. The band frequency value increases as the shade becomes darker. The dark and bright circles indicate the minimum and maximum points, respectively. The details in Figures 3, 4 and 5 are similar to those in Figure 2.

Figure 3. (a) Model of 2D PCs with a rectangular cylinder at the centre of the unit cell; (b-f) Contours of the lowest five eigen-frequencies in the first BZ for (b) band 1, (c) band 2, (d) band 3, (e) band 4 and (f) band 5.

Next, we placed an additional rectangular rod at the centre of the unit cell (Figure 3a, $L_{1x} = L_{1y} = 0.30a$, $L_{2x} = 0.40a$ and $L_{2y} = 0.70a$). The PCs with this configuration have $C_{4v}$ point group symmetry, including four elements. The contours of the phononic band frequencies for the PCs with the unit cell are shown in Figure 3. We examined the distributions carefully from bands 1 (Figure 2b) to 5 (Figure 2f). For band 1, $\omega_{1\text{max}}^{}$ occurs at the centre point $\Gamma$, whereas $\omega_{1\text{min}}^{}$ occurs at corners M, M$_1$, M$_2$ and M$_3$. For band 2, $\omega_{2\text{max}}^{}$ is located at the points of X and X$_1$, whereas $\omega_{2\text{min}}^{}$ is
symmetrically distributed along the lines of $\Gamma X$ and $X_1\Gamma$. For band 3, $\omega_{1\text{min}}^\text{max}$ occurs at
the centre point $\Gamma$, whereas $\omega_{2\text{max}}^\text{max}$ is symmetrically distributed near the lines of $M\Gamma$, $M_1\Gamma$, $M_2\Gamma$ and $M_3\Gamma$. For band 4, $\omega_{3\text{max}}^\text{max}$ is symmetrically distributed along the line of
$\Gamma X$ and $X_1\Gamma$, whereas $\omega_{4\text{min}}^\text{max}$ is symmetrically distributed near the lines of $M\Gamma$, $M_1\Gamma$, $M_2\Gamma$ and $M_3\Gamma$. For band 5, $\omega_{5\text{max}}^\text{max}$ is at the points $M$, $M_1$, $M_2$ and $M_3$, whereas $\omega_{5\text{min}}^\text{min}$ is
located in the areas of $MY\Gamma$, $M_2Y\Gamma$, $M_1Y_1\Gamma$ and $M_2Y_1\Gamma$. We found that the
distribution has four symmetrical operations in the first BZ. Not all extreme points
are in the high symmetry points. In this case, the irreducible BZ must take a quarter of
the first BZ, such as $\Gamma XMY$, before they can obtain the minimum and maximum
points on the entire first BZ and the correct band structures of PCs.

![Figure 4](image)

We placed an additional square rod at (0.30a, 0.30a) of the unit cell (see Figure
4(a), $L_{1x} = L_{1y} = 0.30a$, $L_{2x} = L_{2y} = 0.30a$). The PCs with this configuration have $C_{4v}$
point group symmetry, including two elements. The contours of the phononic band
frequencies for the PCs with the unit cell are shown in Figure 4. We examined the
distributions carefully from bands 1 (Figure 4b) to 5 (Figure 4f). For bands 1 and 2, $\omega_{1\text{min}}^\text{min}$ and $\omega_{2\text{min}}^\text{min}$ occur at the centre point $\Gamma$, whereas $\omega_{1\text{max}}^\text{max}$ and $\omega_{2\text{max}}^\text{max}$ is symmetrically
distributed along the lines of $M\Gamma$ and $M_2\Gamma$. For band 3, $\omega_{3\text{max}}^\text{max}$ is located at the points of
$Y$ and $Y_1$, whereas $\omega_{3\text{min}}^\text{min}$ is symmetrically distributed in $MY\Gamma$ and $M_2Y_1\Gamma$. For band 4, $\omega_{4\text{min}}^\text{min}$ is symmetrically distributed along the lines of $M\Gamma$ and $M_2\Gamma$, whereas $\omega_{4\text{max}}^\text{max}$ occurs at the points $X$, $X_1$, $Y$ and $Y_1$. For band 5, $\omega_{5\text{min}}^\text{min}$ is symmetrically distributed along the
lines of $M\Gamma$ and $M_2\Gamma$, whereas $\omega_{5\text{max}}^\text{max}$ occurs along the lines of $M_1\Gamma$ and $M_3\Gamma$. We found
that the distribution has two symmetrical operations in the first BZ. Not all extreme
points are in the high symmetry points. In this case, the irreducible BZ must take over
half of the first BZ, such as $MM_1M_2$, before they can obtain minimum and maximum
points on the entire first BZ and the correct band structure of PCs.
Finally, we placed an additional rectangular rod at (0.35a, 0.60a) of the unit cell (Figure 5a, $L_{1x} = L_{1y} = 0.30a$, $L_{2x} = 0.40a$ and $L_{2y} = 0.70a$). The PCs with this configuration have $C_{4v}$ point group symmetry, including one element. The contours of the phononic band frequencies for the PCs with the unit cell are shown in Figure 5. We examined the distributions carefully from bands 1 (Figure 5b) to 5 (Figure 5f). For band 1, $\omega_1^{\text{min}}$ occurs at the centre point $\Gamma$, whereas $\omega_2^{\text{max}}$ is symmetrically distributed in areas $M_1Y_1\Gamma$ and $M_3Y_3\Gamma$. For band 2, $\omega_2^{\text{min}}$ occurs at the centre point $\Gamma$, whereas $\omega_2^{\text{max}}$ is symmetrically distributed in the areas of $M_1Y_1\Gamma$ and $M_3Y_1\Gamma$. For band 3, $\omega_3^{\text{max}}$ is symmetrically distributed along the lines of $X\Gamma$ and $X_1\Gamma$, whereas $\omega_3^{\text{min}}$ is symmetrically distributed in the areas $M_1Y_1\Gamma$ and $M_3Y_1\Gamma$. For band 4, $\omega_4^{\text{max}}$ is symmetrically distributed along the lines of $X\Gamma$ and $X_1\Gamma$, whereas $\omega_4^{\text{min}}$ is symmetrically distributed in areas $M_1X\Gamma$ and $M_3X_1\Gamma$. For band 5, $\omega_5^{\text{min}}$ is symmetrically distributed on both sides of $M\Gamma$ and $M_2\Gamma$, whereas $\omega_5^{\text{max}}$ is symmetrically distributed in areas $M_1Y_1\Gamma$ and $M_2Y_1\Gamma$. We studied the distribution of eigen-frequencies in the first BZ. The most extreme points are not on the high symmetric points, and the extreme points of different bands are in different regions. The distribution symmetry of extreme points is significantly decreased. Considering the distribution of extreme value in the first BZ, we need to take over the entire BZ to obtain the correct phononic band structures of the PCs.

In Figure 2, the minimum and maximum frequency values fall on the periphery of the basic triangle. In Figure 3, the obtained minimum and maximum must take a quarter of the first BZ. In Figure 4, extreme points must take over half of the first BZ. In Figure 5, we only need to take over the entire BZ to obtain the correct phononic band structures of the PCs. The symmetry of the PC combination of the scatterers and lattice decreased, whereas the irreducible BZ increased.
CONCLUSION

In summary, we study the effect of point-group symmetry to the irreducible BZ of two-dimensional PCs with the plane-wave expansion method. By adding a rod in the different place of the unit cell of PCs, we adjust and lower its point-group symmetry. We find that some of the minimums or maximums of the bands are not locate at the periphery of the irreducible BZ. In low point-group symmetry PCs, it is needed and important to expand the calculated region to find the minimum and maximum values of the band structure in order to get an accurate band gap.

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REFERENCES