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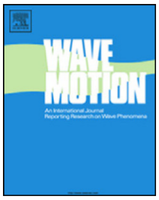

Dispersion analysis with 45°-rotated augmented supercells and applications in phononic crystal design

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HIGHLIGHTS

- The dispersion curves in 45°-rotated augmented supercells are analyzed.
- The effect of the rotation on the Brillouin zone folding is studied.
- Branch overlapping and folding mechanisms in supercells are revealed.
- The overlapping mechanism is utilized for bandgap maximizing topology optimization.

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ABSTRACT

The supercell approach can be useful for tailoring dispersion curves of phononic crystals, but the interpretation of the dispersion curves in the supercells can be often intriguing. Supercells formed by integer multiples of an original unit cell along its lattice axes are common, but there are also important situations requiring supercells formed by non-integer multiples of an original unit cell and its rotation with respect to its lattice axes. In these cases, not only dispersion branch folding, but also branch overlapping not found in common supercells, take place, which complicates the correct interpretation of band structures. In this study, we consider 45°-rotated augmented supercells and analyze why and how branch folding and overlapping take place. For the analysis, the relation between the first Brillouin zone of an original cell and that of the corresponding 45°-rotated augmented supercell is investigated. The analysis of the folding and overlapping mechanism found in the dispersion curve of the supercell is also useful for interpreting which branches can be excited over a target wavevector direction. The usefulness of the findings of this supercell-based dispersion analysis is demonstrated in unit cell design problems. Specifically, we show how to interpret correctly the dispersion curves of phononic crystals made of unit cells optimized by bandgap maximizing topology optimization when the optimized unit cells turn out to be 45°-rotated augmented supercells. Conversely, throughout design optimization iterations, the original period of a unit cell that is initially set at the beginning of design optimization can be maintained if branch overlapping is forced not to occur.

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1. Introduction

Phononic Crystals (PCs) with periodically-arranged inclusions inside a homogeneous host are useful for controlling elastic and acoustic waves. Intrinsic wave phenomena found in PCs, such as bandgap [1–3] and negative refraction [4], can be used for various applications including wave focusing [5], waveguiding [6], wave filtering [7], and wave attenuation [8]. Because the manipulation of these wave phenomena is closely related to the manipulation of dispersion curves, accurate analysis of dispersion curves is important. In addition, tailoring of dispersion curves by varying various PC parameters such as material property, lattice symmetry, resonator shape, and rotation of inclusions has been an active field of study [9–16]. Especially when parameter studies involve the periods of PC unit cells, dispersion analysis with the supercell approach can be effective. A two-dimensional supercell is typically an augmented unit cell consisting of $n \times m$ ($n,\ m =$ positive integer) times the original unit cell. In this case, the directions of lattice axes are assumed to be unaltered. Earlier studies explain how to interpret the dispersion curves plotted by the supercell approach [17,18]. If unit cell axes are also allowed or made to rotate as a result of parameter changes (in two or higher-dimensional cases only), which is the subject of this study, the required supercell is not only augmented and but also rotated. Because of the axis rotation, the dispersion curves plotted with respect to an augmented, rotated supercell will look quite different from and become much more complicated than those plotted with respect to an augmented supercell without rotation.

As an example of the dispersion curve plotted with a rotated augmented supercell, let us consider Fig. 1. Fig. 1(a) shows a two-dimensional PC consisting of square unit cells with inclusions. As a design problem, one can consider altering band structures by changing the size of inclusions. Specifically, the square unit cell is to be optimized in which defined by the square dotted line in Fig. 1(a). The 4 corner quadrants can vary in size (radius) while the central circular inclusion remains unchanged. If the radius of the 4 quadrants becomes equal to the radius of the central circular inclusion, Fig. 1(b) turns out to be the correct unit cell for the corresponding dispersion analysis. In this case, the unit cell shown in Fig. 1(c) can be viewed as a 45°-rotated augmented supercell compared with the true unit cell in Fig. 1(b). As a result, the dispersion curves plotted in Fig. 1(c) become quite complicated and have overlapping branches over a range of wavevectors. In addition, it has been reported in practical engineering PC design studies that a 45°-rotated augmented supercell could be obtained as the results of optimization [19–23]. However, the analysis of the dispersion curve in a rotated augmented supercell requires further exploration. Our aim is to fully analyze the dispersion curve in a 45°-rotated augmented square supercell.

This paper is organized as follows. In Section 2, we reveal how the dispersion curves plotted with respect to the supercell match those plotted with respect to the original unit cell. In doing so, we also show that non-propagating branches appear in a certain wavevector region. Furthermore, we show how branch overlapping takes place in the supercell-based dispersion curves. To gain some insight, we employ a graphical approach by comparing the 1st Brillouin Zone (BZ) of the supercell with that of the original unit cell. Once the characteristics and origins of the dispersion curves plotted with respect to the supercell are analyzed, wave propagation in a PC structure can be correctly interpreted.

In Section 3, we show how the findings in Section 2 can be utilized in practical PC design problems, especially for bandgap maximizing topology optimization problems. Through these problems, it can be demonstrated that the correct analysis of the dispersion curve in a 45°-rotated augmented supercell is important not only in the interpretation of optimized results but also in keeping the initially-set periodicity throughout optimization iterations.

2. Dispersion analysis in the 45°-rotated augmented supercell

Fig. 1(a) shows a two-dimensional PC, the unit cell of which is a square unit cell $\boldsymbol{C}$ of size $d_u = d/\sqrt{2}$, and the lattice vectors ($\boldsymbol{e_1},\ \boldsymbol{e_2}$). The dispersion curves for the PC, analyzed with respect to $\boldsymbol{C}$, are shown in Fig. 1(b) and were obtained by the finite element method for two-dimensional in-plane waves consisting of longitudinal-dominant and shear-dominant motions. For instance, the lowest and the second lowest branches appearing along Γ–X (see the definition of these symbols in Fig. 2(b)) denote the shear-dominant ("*SH-dominant*") and longitudinal-dominant ("*L-dominant*") wave modes, respectively. The PC in Fig. 1(a) is made of an aluminum ($E = 70$ GPa, $\upsilon = 0.34$, $\rho = 2700$ kg/m^3) host and circular tungsten ($E = 360$ GPa, $\upsilon = 0.27$, $\rho = 17,800$ kg/m^3) inclusions of radius $0.3d$. Here, Young's modulus and Poisson's ratio are denoted by E and υ, respectively. For subsequent numerical analyses, $d = 0.02$ m is used.

As we attempt to analyze the dispersion curve of the same PC with respect to a 45°-rotated augmented supercell $\boldsymbol{C}_{\boldsymbol{S}\text{-}\boldsymbol{45}^\circ}$ of $d_s = d$, lattice vectors $\boldsymbol{e_{1S}}$ and $\boldsymbol{e_{2S}}$ ($|\boldsymbol{e_{1S}}| = |\boldsymbol{e_{2S}}| = d_s$) are introduced. If the Cartesian axes are assumed to be aligned with $\boldsymbol{e_{1S}}$ and $\boldsymbol{e_{2S}}$, then $\boldsymbol{e_{1S}} = (d, 0)$, $\boldsymbol{e_{2S}} = (0, d)$, $\boldsymbol{e_1} = (d, d)/2$, and $\boldsymbol{e_2} = (-d, d)/2$. Fig. 1(c) shows the dispersion curves analyzed with respect to the supercell $\boldsymbol{C}_{\boldsymbol{S}\text{-}\boldsymbol{45}^\circ}$. These curves appear quite complicated in comparison with those shown in Fig. 1(b), analyzed with respect to $\boldsymbol{C}$.

To analyze the dispersion curves in the wavevector spaces corresponding to $\boldsymbol{C}$ and $\boldsymbol{C}_{\boldsymbol{S}\text{-}\boldsymbol{45}^\circ}$, the reciprocal lattice vectors for $\boldsymbol{C}$ and $\boldsymbol{C}_{\boldsymbol{S}\text{-}\boldsymbol{45}^\circ}$ are introduced in Fig. 2(a): $\boldsymbol{b_1} = 2\pi/d(1, 1)$, $\boldsymbol{b_2} = 2\pi/d(-1, 1)$ for $\boldsymbol{C}$, $\boldsymbol{b_{1S}} = 2\pi/d(1,\ 0)$, and $\boldsymbol{b_{2S}} = 2\pi/d(0, 1)$ for $\boldsymbol{C}_{\boldsymbol{S}\text{-}\boldsymbol{45}^\circ}$. The 1st BZs corresponding to $\boldsymbol{C}$ and $\boldsymbol{C}_{\boldsymbol{S}\text{-}\boldsymbol{45}^\circ}$ are plotted in Fig. 2(b) with the reciprocal lattice vectors illustrated. Note that the 1st BZ of $\boldsymbol{C}$ completely encloses the 1st BZ of $\boldsymbol{C}_{\boldsymbol{S}\text{-}\boldsymbol{45}^\circ}$. However, the orientations of $\boldsymbol{b_{1S}}$ and $\boldsymbol{b_{2S}}$ are different from those of $\boldsymbol{b_1}$ and $\boldsymbol{b_2}$. Therefore, the dispersion curves plotted with respect to the supercell $\boldsymbol{C}_{\boldsymbol{S}\text{-}\boldsymbol{45}^\circ}$ require careful interpretations different from those for a one-dimensional supercell or two-dimensional augmented supercell without unit cell rotation. Such complexity in interpreting the dispersion curves with respect to $\boldsymbol{C}_{\boldsymbol{S}\text{-}\boldsymbol{45}^\circ}$ comes from the cell rotation. We pay special