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Band Structure Design for a Two-Dimensional Phononic Crystal using Various Optimization Methods

様々な最適化手法を用いた２次元フォノニック結晶のバンド構造最適化

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1. Introduction

Phononic crystal(1) is an artificial structure in which materials with different sound velocities and densities are periodically arranged. It has features such as forming a band gap in the dispersion diagram and blocking sound wave propagation in that frequency band. By introducing defects in a part of the crystal, a localized mode appears in the band gap, and an acoustic waveguide that operates selectively at the frequency can be engineered by designing the band structure. Here we focus on a two-dimensional phononic crystal aiming to design high-efficiency acoustic waveguides. In most of previous studies of phononic crystals, including ours, the unit cell structure, especially its symmetry, has been selected empirically and/or heuristically. The band structure of phononic crystals has then been optimized by adjusting the structural parameters before an actual fabrication. In the present study, we aim to develop an optimization algorithm that searches(2) for the desired phonon band structure computationally. The search for an optimum band structure and a corresponding eigenmode involves complex processes, that is, the real space parameter search for optimum properties in the reciprocal space. The applicability of existing algorithms to this problem has been elusive until now. Here we examine the efficiency of some representative metaheuristic algorithms, *i.e.* the Metropolis Monte Carlo method, the shape optimization method, and the topology optimization method are performed. We focus on maximizing the phonon band gap between the first and second bands for entire k-space, at X-point, and M-point.

2. Optimization method

First, we searched for the optimum structure using the Metropolis Monte Carlo (MC) method. The MC algorithm is developed to search for the optimum solution through a stochastic evolution in the parameter space. In general, the MC method can fall into a local minimum. Also the optimum value obtained may differ depending on the temperature setting during the annealing and quenching processes.

Next, we examine a structure search using the shape optimization method. The shape optimization is a method in which the boundary line is used as a design variable and the search is performed by continuous deformation of the boundary line. Since it does not include random selection of structural elements, it is possible to efficiently obtain a more appropriate solution. However, it is known that the optimum structure obtained in the shape optimization method largely depends on the initial shape. Therefore, we verify the optimization process from some randomly selected initial structures.

Finally, optimization is performed using the topology optimization method. The topology optimization(3)(4)(5) involves structural evolutions incorporating the "phase", which represents the number of holes in the structure, into the design variables. Since the optimization can be performed by changing the number of holes and/or of folding of the shape, the degree of freedom in searching space is higher than that of the shape optimization method, expecting higher efficiency for the present purpose.

2. Results

The optimization process by the MC method is shown in **Fig. 1**. The structure was optimized through a deformation process that was close to continuous from the boundary with the surrounding media, and the value of the normalized bandgap converged around 0.88. Here the normalized frequency is defined as $\tilde{f} \equiv fa/c$, where f, a, c represent respectively frequency, lattice constant of the periodic cell, and sound velocity of the background media. There is a high possibility, however, that it is trapped at the local solution within the region of the complex structure in the parameter space. The improvements such as adding constraints to the search space are thus necessary.

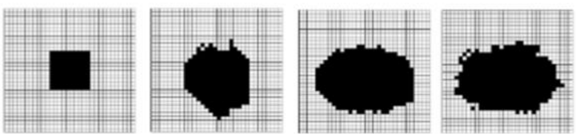

Fig.1 Structural changes during the MC step with a boundary constraint.

Next, the result of the structural search that maximizes the bandgap by the shape optimization algorithm is shown in **Fig. 2**. The figure indicates that the optimization is evolved along the boundary line. We examined the optimization process starting with several initial structures selected. Here, we optimized from 10 different rectangles with arbitrary choices of aspect ratios and compared the final structures. In each case, the normalized bandgap converged to 0.9196 with an identical structure.

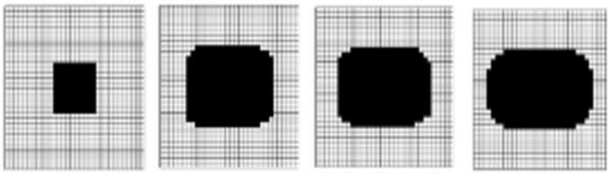

Fig.2 Structural change using shape optimization.

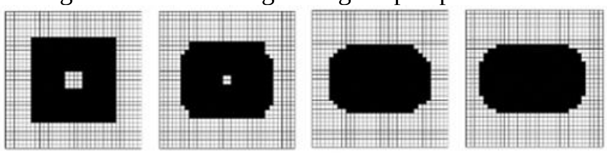

Fig.3 Topology optimization with one hole.

Finally, structural search using the topology optimization was performed. Here, we adopted the topology optimization with a simple algorithm, in which some holes were made in the initial structure and subsequently the shape optimization process was performed. As a result of optimizing from the structure with single hole at the center, as shown in **Fig. 3**, the hole closed during the optimization, resulting in the same process as the shape optimization without holes, and eventually converged to an identical structure. Since there is a possibility that the holes might have closed accidentally, an additional calculation was also performed with increasing the number and size of holes in the initial structure. Nevertheless, the holes are all closed during the optimization also in this process. It thus turned out to be an optimum structure.

In the above examinations, the structure of the phononic crystal has been optimized from the band calculation along the path between the high symmetry points of the reciprocal lattice space so that the value of the lowest bandgap is maximized for all the wave number. Here, we also examine a bandgap optimization for specific directions in k-space. The search for the maximum bandgap at points X and M in the reciprocal space were performed using the methods of the shape optimization and the topology optimization. **Figures 4** and **5** show the optimization process for shape optimization at X- and M-points.

For the X-point maximization both methods had given the same results as an optimum structure. For the M-point maximization, on the other hand, the results of topology optimization fell into local solutions in the vicinity of each initial structure.

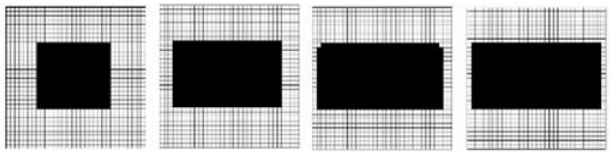

Fig.4 Shape optimization for X-point maximization.

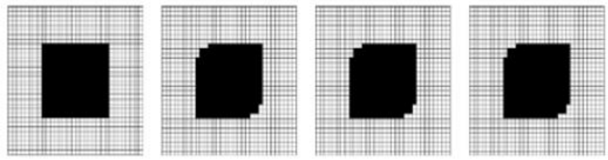

Fig.5 Shape optimization for M-point maximization

3. Conclusion

While the structural search using the MC method could not find the optimum solution for the lowest full bandgap in the phononic dispersion diagram, it was successfully optimized by using the shape optimization method and the (simplified) topology optimization method. Also, from the bandgap optimization on the M and X points in the reciprocal lattice space, it was found that the optimized structure of the bandgap is significantly different for each specific direction of k-space. From these findings, it will be possible to design a phononic waveguide model where a localized gap mode can propagate efficiently by suppressing a possible scattering and diffusion along the paths of the waveguide. Development of an algorithm that optimizes the mode shape in the phonon band, as well as a topological invariance (Chern number) related to the band topology in the wave number space is in progress.

References

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