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Structural Inverse Design of 2D Phononic Crystals using Deep Learning Model

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1. Introduction

In the design of phononic crystals (PnCs) [1)], many studies have focused on maximizing size of the band gap (BG) through various optimization methods such as topology optimization[2)], Monte Carlo simulations[3)], and other evolutionary algorithms[4)]. On the other hand, "inverse problem approaches" to identify materials and structures of PnCs that achieves a desired BG frequency and size is difficult without prior knowledge on which material properties of choices affect predominantly. In recent years, with the advancement of artificial intelligence technology, new approaches applying machine learning are attracting much attention. However, simple machine learning can only solve the forward problem of predicting the frequency range and size of BG from a specific PnCs, whereas the inverse problem of determining the PnCs structure and materials that yield a specific BG frequency and size is a complex black-box optimization problem that can often be unsolvable. The relationship between the forward and inverse problems of machine learning is shown in **Fig. 1**. In this study, we developed a methodology for solving the inverse problem using deep learning model to achieve the structural inverse design of PnCs that yield a desired BG frequency and size.

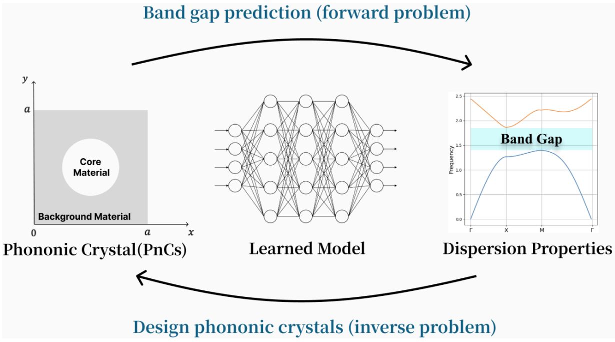

Fig. 1 Relationship between forward and inverse problems in PnCs and BG applying deep learning model

2. Data Preparation

In this study, we consider two-dimensional PnCs with a square lattice consisting of a background material and a central material. **Figure2** shows a plan view of PnCs in which the central material is a cylinder and a square pillar [5)].

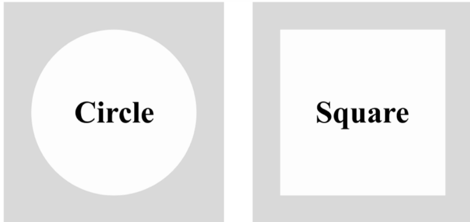

Fig. 2 Plan view of 2D PnCs with a cylindrical (left) and a square pillar (right) embedded in the background material

The dispersion properties have been calculated by solving the wave equation of the elastic body based on the plane wave expansion method. In order to confirm the applicability of machine learning, this study uses a model equation that can represent elastic wave propagation only with transverse waves in a solid material without anisotropy. In collecting the training data, the elastic modulus, density, filling fraction, and shape of the central material were varied while the elastic modulus and density of the background material were normalized to 1. Additionally, to broaden the data range, calculations were also performed for structures with the shape obtained by combining cylindrical and square pillars, as shown in **Fig. 3**.

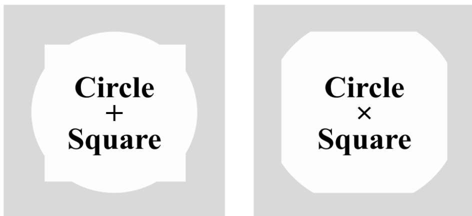

Fig. 3 Combining schemes of the shapes of central material in 2D PnCs: addition (left) and multiplication (right)

3. Structural Design by Inverse Problem using Deep Learning Model

We then constructed a deep learning model, and as a result of learning, we achieved high performance in forward prediction of the BG, with a coefficient of determination(R^2) of 0.99. **Figure4** shows an image of the constructed deep learning model. The input data are the elastic modulus(C), density(ρ), filling

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fraction(f), and structural parameters(s) of the central material in the PnCs, and the output data are the lower band edge(ω_1_min) and the size of the BG(BG_size).

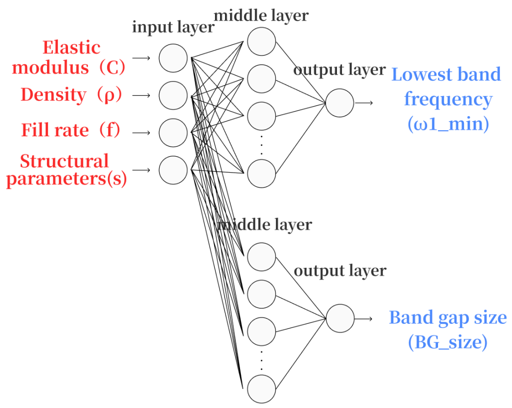

Fig. 4 Image of the constructed deep learning model

This learned model $g()$ was then applied for the structural inverse design of PnCs. To achieve this, the desired ω_1_min, BG_size and the squared error of the predicted data generated by the deep learning model were set as the objective function defined as in Eqs.(1) and (2).

$$f_{\omega 1\_\mathrm{min}} = \left(g(C,\rho,f,s) - \mathrm{target}_{\omega 1\_\mathrm{min}}\right)^2 \qquad (1)$$

$$f_{\mathrm{BG\_size}} = \left(g(C,\rho,f,s) - \mathrm{target}_{\mathrm{BG\_size}}\right)^2 \qquad (2)$$

Thus, by setting up an objective function applying the learned model called $g()$, the problem can be regarded as in the framework of mathematical optimization. By minimizing each objective function, the values one wishes to find can be obtained as the solution. This is a multi-objective optimization problem using deep learning model, and the inverse problem can be solved by using gradient descent algorithm [6], group intelligence [7], and evolutionary algorithms[8] to search for the pareto solution and pareto front as illustrated in **Fig. 5**.

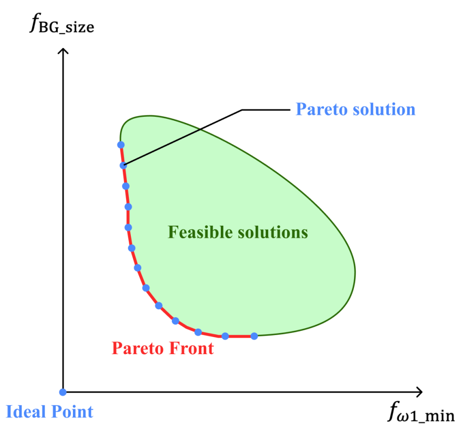

Fig. 5 Concept of multi-objective optimization

4. Result

By applying a genetic algorithm (NSGA-II) to solve a multi-objective optimization problem, we confirmed that the structural inverse design of PnCs has successfully derived the desired outcomes. As a result, we could design the desired PnCs for various targets of ω_1_min and BG_size with error rates as low as 0.01%. For instance, when targeting ω_1_min$:= 1$ and BG_size$:= 0.4$, the structural inverse design yielded PnCs with ω_1_min ≈ 1.005 and BG_size ≈ 0.4023, as shown in **Fig. 6**.

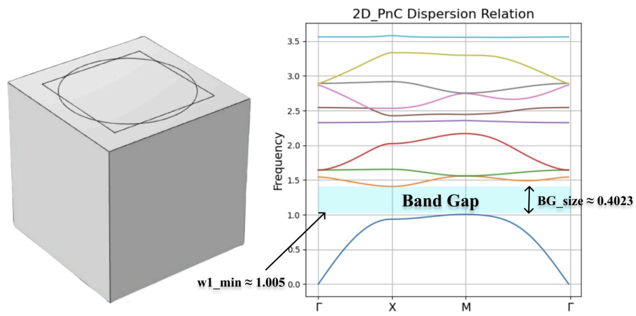

Fig. 6 Structure and its dispersion obtained by the present inverse design algorithm of PnCs

5. Conclusion

We solved a multi-objective optimization problem by applying a deep learning model to perform the structural inverse design of 2D PnCs for obtaining desired BG frequency and size. As a result, we confirmed that the desired PnCs could be designed within an error rate of 0.01% across a wide ranges of problem setting. Details of the algorithm as well as future perspective of the developed method will be given in the presentation.

References

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