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Topological design of pentamode lattice metamaterials using a ground structure method

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HIGHLIGHTS

• A general mathematical formulation is proposed for design of three-dimensional pentamode metamaterials with at least orthotropic symmetry.
• A ground-structure topology optimization method with the genetic algorithm is proposed for inverse design of pentamode lattices.
• Geometric constraints on intersection and overlap of bars are imposed on design optimization of truss-like lattices.
• Twenty-four new pentamode lattices are discovered, including isotropic, transverse isotropic and orthotropic.

ABSTRACT

Pentamode metamaterials are a new class of artificially engineering three-dimensional lattice composites. There exist a few types of pentamode metamaterials that are dominated by ad hoc design motifs, while a systematic design approach is still missing. This paper will present an efficient topological optimization methodology to discover a series of novel pentamode lattice microarchitectures over a range of effective material properties. Firstly, the necessary and sufficient condition that is required for elasticity constants of pentamode micro lattices with at least elastically orthotropic symmetry is derived. Secondly, a general mathematical formulation for design optimization of such pentamode micro lattices is developed. Thirdly, a truss-based three-dimensional ground structure with geometrically orthotropic symmetry is generated, with geometric constraints to avoid intersection and overlap of truss bars within the ground structure. The genetic algorithm is then used to solve the topology optimization problem described by the ground structure. Finally, twenty-four pentamode lattices are designed to demonstrate the effectiveness of the proposed method.

1. Introduction

Pentamode metamaterials belong to a kind of three-dimensional solid mechanical metamaterials that are artificially architected to only bear single mode of stress [1]. A pentamode metamaterial only has one non-zero eigenvalue from its sixth-order elasticity matrix, and therefore it can deform easily in five independent modes corresponding to five zero eigenvalues from its elasticity matrix [1,2]. Take an isotropic pentamode metamaterial as an example, it has a finite bulk modulus but a vanishing shear modulus and can only bear hydrostatic stress. In other words, they are three-dimensional lattice microstructures engineered
to mimic the behavior of fluids. The unusual mechanical properties of pentamode metamaterials are gained from the geometries of their rationally designed microarchitectures, rather than the chemical compositions of their base materials (e.g., metals and polymers).

The pentamode metamaterial was first designed by Milton and Cherkaev in 1995 [1]. They are dominantly featured with a diamond-type lattice, consisting of four double-cone rigid-body bars that are jointed only at their point-like tips [1]. However, lattice microarchitectures with such point-like tips cannot stably exist in real-world applications. The infinitely small joints were therefore given finite cross-sections to facilitate manufacturing of the pentamode lattices in practice [3]. This conventional diamond-type pentamode lattice [3] is illustrated in Fig. 1a, having a smaller diameter d at the joints, a relatively large diameter D at the midspan and a total length l of a double-cone bar as shown in Fig. 1b. For the double-cone lattice, the work [4] showed that using asymmetric double-cone bars can increase the ratio of the bulk modulus to the shear modulus. Huang et al. [5] quantitatively compared the pentamode behavior and acoustic bandgaps of the diamond-type pentamode lattices with five different cross-sectional shapes, and found that the triangle case performs best with lower frequency and broader bandwidth than other four shapes.

Isotropic pentamode metamaterials can uncouple the compression wave and shear wave, as ideally the bulk moduli can be infinitely large compared to the shear moduli [3]. In other words, they are difficult to compress while easily flow away, for which they are also named as metafluids [6]. Kadic et al. [3] should be the first group implemented a pentamode lattice using dip-in direct-laser-writing optical lithography. The testing results of the manufactured diamond-type metal pentamode lattices revealed that the shear and Young’s moduli are in good agreement with their theoretical calculations [7], and the elastic modulus and yield stress were decoupled from the relative density [8].

Pentamode metamaterials are promising for transforming elastostatics and particularly elastodynamics to enable acoustic cloaks [9–15], based on the concept of transformation optics but beyond that. In 2008, Norris [9] investigated the transformation acoustic cloaks and noted that ideal acoustic cloaks can be achieved through pentamode metamaterials. Compared with conventional inertial cloaks, pentamode acoustic cloaks can avoid mass singularity and be engineered with pure solid materials and are theoretically broadband since they invoke only quasi-static stiffness of pentamode metamaterials [12]. Potential applications of pentamode metamaterials in other fields have also been studied recently. For instance, Buckmann et al. [16] designed an elasto-mechanical unfeelable cloak using the conventional diamond-type pentamode metamaterials to hide hard objects and make them unfeelable. Hai et al. [17] used bimodal structures to design two-dimensional unfeelable mechanical cloaks to reduce the influence of a hole in the structure on stress concentrations and redistribute the strain. Fabbricino et al. [18] proposed a tunable seismic base-isolation device by the combination of pentamode lattices and tensegrity structures.

It is noted that several ‘pentamode metamaterials’ given in literatures [11–14] are actually two-dimensional bimode metamaterials. Strictly speaking, they should have not been classified as pentamode metamaterials because three-dimension with sixth-order elasticity matrices is a necessity to define the term of penta referring to five. Of cause, a pentamode metamaterial can be considered as a three-dimensional extension of a two-dimensional bimode honeycomb metamaterial that has three linkages meet at a point. Therefore, Morse and Cherkaev [1] noted that a natural candidate might have four linkages meet at a point, which helped to discover the diamond-type pentamode lattices. Inspired by the concept of the Bravais lattices, Mejica and Lantada [19] presented a library of lattices claimed to be pentamode in 2015, but Xu [20] stated that although these lattices are not pentamode although have large ratios of the bulk modulus to the shear modulus. This phenomenon will be explained in Section 2 of this paper. In 2015, Xu [20] presented five pentamode lattices that all have only one non-zero eigenvalue from the effective elasticity matrix. In 2019, Li and Vipperman [21], and Huang et al. [22] further proposed two isotropic pentamode lattices. From the above, we can find that seven new pentamode lattices have been found but through ad hoc and empirical design methods since 1995. A generative design optimization approach that can systematically discover a range of novel pentamode lattices over a wide scope of effective properties is still missing.

Milton and Cherkaev [1] noted that pentamode metamaterials can be anisotropic. However, this possibility was not addressed and come into reality until 2013, when Kadic et al. [23] introduced intentional anisotropy into the conventional diamond-type lattices by moving just one connection point along the space diagonal. As mentioned by Milton et al. [24], pentamode metamaterials should be able to bear any chosen stress, not only isotropic. Anisotropic pentamode metamaterials are the prerequisite for realizing many applications including acoustic cloaks based on transformation elastodynamics [23]. Hence, this work will focus on topology optimization of more general pentamode metamaterials not limited to isotropic. An evolutionary ground structure method using the genetic algorithm is proposed to discover novel pentamode lattice microstructures with at least orthotropic symmetry.

2. Necessary and sufficient condition

This section will rigorously derive the necessary and sufficient condition required for elasticity matrices of pentamode metamaterials with at least orthotropic symmetry. It is noted that the derivation here is valid for linear elasticity. For three-dimensional elasticity problem,

---

**Fig. 1.** Diamond-type pentamode lattice with double-cone bars.
Hooke’s law is here considered in the form $\mathbf{C} = \mathbf{C}_0$, where $\mathbf{C}$ is the vector of stress, and $\mathbf{e}$ is the vector of strain. For any elastic matrix with orthotropic symmetry, the elasticity matrix $\mathbf{C}$ is defined in Eq. (1). It is noted that an elasticity matrix is always positive semidefinite, i.e., $\mathbf{C} \succeq 0$, where $i = 1, 2, 3, 4, 5, 6$.

$$
\mathbf{C} = \begin{bmatrix}
C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\
C_{22} & C_{23} & 0 & 0 & 0 & 0 \\
C_{33} & 0 & 0 & 0 & 0 & 0 \\
C_{44} & C_{55} & C_{66} & 0 & 0 & 0
\end{bmatrix} \tag{1}
$$

The essential definition of a pentamode metamaterial is that it has only one non-zero eigenvalue from its sixth-order elasticity matrix [1,9]. The characteristic polynomial of the elasticity matrix in Eq. (1) can be defined as:

$$
|\mathbf{C} - \lambda \mathbf{I}| = (C_{44} - \lambda)(C_{55} - \lambda)(C_{66} - \lambda)(A_1 + (A_2 + (A_3 - \lambda)\lambda)\lambda) = 0 \tag{2}
$$

where

$$
\begin{align*}
A_1 &= C_{11}C_{22}C_{33} + 2C_{12}C_{13}C_{23} - C_{11}C_{23}^2 - C_{12}C_{13}^2 - C_{23}C_{11}^2 \\
A_2 &= C_{12}^2 - C_{11}C_{22} + C_{13}^2 - C_{11}C_{33} + C_{23}^2 - C_{22}C_{33} \\
A_3 &= C_{11} + C_{22} + C_{33}
\end{align*} \tag{3}
$$

To find the necessary and sufficient condition for this characteristic polynomial to have only one non-zero root, we should consider through two different cases.

The first case is that at least one of $C_{44}$, $C_{55}$ and $C_{66}$ is positive, e.g., $C_{44} > 0$. If so, the only non-zero eigenvalue should be $\lambda = C_{44}$, and then the following conditions must be satisfied:

$$
\begin{align*}
C_{55} &= C_{66} = 0 \\
A_1 = A_2 &= A_3 = 0
\end{align*} \tag{4}
$$

Since the elasticity matrix is positive semidefinite, the second equation in Eq. (4) equals to the following condition:

$$
C_{11} = C_{22} = C_{33} = C_{12} = C_{13} = C_{23} = 0
$$

The derivation for $C_{55} > 0$ or $C_{66} > 0$ is the same. Therefore, the general necessary and sufficient condition for this first case is that only one of $C_{44}$, $C_{55}$ and $C_{66}$ is positive while all other elastic constants are zero, which corresponds to a lattice that can only bear one shear stress mode, which is well in line with the definition of pentamode metamaterials in [1].

It is noted that in this paper we will only consider the second case described below for design optimization since it is more complicated and physically meaningful. The second case is that at least one of $C_{11}$, $C_{22}$ and $C_{33}$ is positive. If so, the only non-zero eigenvalue should be $\lambda = A_3 = C_{11} + C_{22} + C_{33}$, and then the following conditions must be satisfied:

$$
\begin{align*}
C_{44} &= C_{55} = C_{66} = 0 \\
A_1 = A_2 &= 0
\end{align*} \tag{6}
$$

For the equation $A_3 = 0$ in Eq. (6) to have three real roots as $C_{12}, C_{13}$ and $C_{23}$, from mathematical knowledge we can know that the following conditions must be satisfied:

$$
\begin{align*}
4C_{11}^2C_{23}^2 - 4C_{12}^3C_{13} - 4C_{22}C_{12}C_{13}^2 - C_{11}C_{23}^2 &\geq 0 \\
4C_{12}^2C_{23}^2 - 4C_{12}^3C_{13} - 4C_{22}C_{12}C_{13}^2 - C_{11}C_{23}^2 &\geq 0 \\
4C_{12}^2C_{13}^2 - 4C_{11}C_{22}C_{12}C_{13}^2 - C_{11}C_{23}^2 &\geq 0
\end{align*} \tag{7}
$$

which can be simplified as:

$$
\begin{align*}
\begin{cases}
C_{12}^2C_{13} - C_{11}C_{23} &\geq 0 \\
C_{12}^2C_{13} - C_{11}C_{23} &\geq 0 \\
C_{12}^2C_{13} - C_{11}C_{23} &\geq 0
\end{cases}
\end{align*}
$$

These inequality equations require the values of $C_{12}^2 - C_{11}C_{23}$, $C_{12}^2 - C_{11}C_{23}$ and $C_{12}^2 - C_{11}C_{23}$ to have no opposite signs. Combined with the equation $A_2 = 0$ in Eq. (6), we can know that the following condition must be satisfied:

$$
C_{12}^2 - C_{12}C_{23} = C_{13}^2 - C_{11}C_{23} = C_{23}^2 - C_{22}C_{33} = 0
$$

which can be simplified to:

$$
\begin{align*}
C_{12} &= a\sqrt{C_{11}C_{22}} \\
C_{13} &= b\sqrt{C_{11}C_{33}} \\
C_{23} &= c\sqrt{C_{22}C_{33}}
\end{align*} \tag{8}
$$

where

$$
a = \pm 1, b = \pm 1, c = \pm 1
$$

Moreover, from the equation $A_3 = 0$ in Eq. (6), we can know that:

$$
C_{11}C_{22}C_{33} + 2C_{12}C_{13}C_{23} = (1 + 2abc)C_{11}C_{22}C_{33}
$$

which can be simplified as:

$$
\begin{align*}
\begin{cases}
C_{11}a\sqrt{C_{11}C_{22}} &\geq 0 \\
C_{22}b\sqrt{C_{22}C_{33}} &\geq 0 \\
C_{33}c\sqrt{C_{33}} &\geq 0
\end{cases}
\end{align*}
$$

where

$$
a = b = c = 1
$$

It is noted that the condition above also contain the case that only one of $C_{11}$, $C_{22}$ and $C_{33}$ is positive while all other elastic constants are zero. Therefore, the necessary and sufficient condition required for elastic materials with at least orthotropic symmetry to be pentamode for the second case is the combination of Eqs. (10), (14) and the equation $C_{44} = C_{55} = C_{66} = 0$ in Eq. (6). When satisfying this necessary and sufficient condition, the elasticity matrix can be simplified as:

$$
\begin{bmatrix}
C_{11} & a\sqrt{C_{11}C_{22}} & 0 & 0 & 0 & 0 \\
C_{22} & b\sqrt{C_{22}C_{33}} & 0 & 0 & 0 & 0 \\
C_{33} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
$$

The corresponding eigenvector of the only one non-zero eigenvalue $\lambda = C_{11} + C_{22} + C_{33}$ is:

$$
\mathbf{x} = \begin{bmatrix}
ad\sqrt{C_{11}} & ac\sqrt{C_{22}} & bc\sqrt{C_{33}} & 0 & 0 & 0
\end{bmatrix}^T
$$

As mentioned above, a pentamode metamaterial has only one non-zero eigenvalue from its sixth-order elasticity matrix [1,9]. It indicates that there are five independent strain cases that each strain case or
their linear combinations will produce zero stress and zero strain energy [6]. It also indicates that this kind of materials can only bear single mode of stress, corresponding to the non-zero eigenvalue [1]. As a special case, isotropic pentamode metamaterials must have the following type of elasticity matrix:

\[
\mathbf{C} = \begin{bmatrix}
C_{11} & C_{11} & C_{11} & 0 & 0 & 0 \\
C_{11} & C_{11} & 0 & 0 & 0 & 0 \\
C_{11} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\]  

(17)

For the above elasticity matrix, there is only one non-zero eigenvalue \( \lambda = 3C_{11} \), and its corresponding eigenvector is \( [1 \ 1 \ 1 \ 0 \ 0 \ 0] \). We can find that this non-zero eigenvalue is exactly three times the bulk modulus \( B = C_{11} \), and the eigenvector indicates that the material can only bear the hydrostatic stress. Therefore, isotropic pentamode metamaterials are equivalently identified by a finite bulk modulus and a vanishing shear modulus [3,7]. However, it is not applicable to non-isotropic pentamode metamaterials. For pentamode metamaterials with at least orthotropic symmetry, we can find that the non-zero eigenvalue \( \lambda = C_{11} + C_{22} + C_{33} \) is not always proportional to its bulk modulus in Eq. (18), and the eigenvector in Eq. (16) does not always correspond to hydrostatic stress either.

\[
B = \frac{C_{11}C_{22}^2 + C_{22}C_{13}^2 + C_{33}C_{12}^2 - 2C_{12}C_{13}C_{23} - C_{11}C_{22}C_{33}}{C_{12}^2 + C_{13}^2 + C_{23}^2 + 2(C_{12}C_{23} + C_{22}C_{13} + C_{33}C_{12} - C_{12}C_{13} - C_{13}C_{23} - C_{23}C_{12}) - (C_{11}C_{22} + C_{11}C_{33} + C_{22}C_{33})}
\]

(18)

Therefore, a relatively very large ratio of the bulk modulus to the shear modulus is no more a sufficient condition for non-isotropic pentamode metamaterials. In other words, such a ratio cannot be used to identify whether an orthotropic or transverse isotropic lattice is a pentamode or not. In Mejica and Lantada [19], for example, although the lattices have large ratios of the bulk modulus to the shear modulus, they are not isotropic and their elasticity matrices have more than one non-zero eigenvalues [20].

3. Genetic-algorithm-based ground structure method

In this section, we propose a topology optimization method to discover novel pentamode lattices with at least orthotropic symmetry. Topology optimization is a powerful design tool able to find novel structures and materials. It is essentially a numerical process to iteratively re-distribute materials within a design domain to find the best distribution with optimized objective performance subject to a set of prescribed constraints. Topology optimization methods of continuum structures, e.g. density-based method, level set method and evolutionary structural optimization method, have been applied to design metamaterials [25-28]. For discrete structures, the most popular topology optimization method should be the ground structure method, which has also been applied in design optimization of mechanical metamaterials [29-31].

Since potential pentamode lattices to be designed in this paper have nearly zero effective shear moduli, it is expected that these lattices should behave like mechanisms and consist of hinge-type joints. However, it is difficult to obtain an optimized design with hinge joints when topology optimization methods of continuum structures with the solid finite elements are used. Hence, we will propose a ground structure method for design of pentamode metamaterials, using truss elements in the numerical homogenization of lattices.

3.1. Optimization formulation

We assume that there is a truss structure with a fixed number of bars, termed as the ground structure. The active bars in the ground structure are chosen as design variables. The finally designed lattice is then formed by active bars. Using the finite element method and the numerical homogenization method, the effective elasticity matrix \( \mathbf{C}^H \) of the lattice can be calculated by:

\[
\mathbf{C}^H = \frac{1}{V} \mathbf{U}^T \mathbf{K} \mathbf{U}
\]

(19)

where \( V \) is the volume of the lattice, \( \mathbf{K} \) is the global stiffness matrix of the structure. The displacement fields \( \mathbf{U} \) in six load cases are calculated with the following periodic boundary condition. For every two points \( p \) and \( q \) that are periodically coincident on the lattice’s boundaries, their nodal displacements \( \mathbf{u} \) must satisfy the following equation:

\[
\mathbf{u}(x_p) - \mathbf{u}(x_q) = \mathbf{e}^p (x_p - x_q)
\]

(20)

where \( x \) is the point coordinate, and \( \mathbf{e}^p \) is the prescribed macroscopic strain of the \( p \)-th load case. For each load case, only one strain component is set to unit whereas the rest five as zero. In other words, the prescribed macroscopic strains for the six load cases are \( \mathbf{e}^p = \mathbf{I} \). To prevent rigid body motions, displacements of one arbitrary point should be fixed. For theoretical and numerical implantation details of the typical numerical homogenization method, readers may refer to [32].

After obtaining the homogenized effective elasticity matrix, we should establish a fitness function to justify whether it satisfies the necessary and sufficient condition derived in Section 2 for pentamode metamaterials with at least orthotropic symmetry. Firstly, for metamaterials with at least orthotropic symmetry, it is obvious that the tension-shear coupling terms in the elasticity matrix must be zero. We exclude that these terms from the objective function and treat them as equality constraints in the mathematical model, because they can be strictly satisfied by guaranteeing that the ground structure has the geometrically orthotropic symmetry. Secondly, we rewrite the Eq. (10) as the following form:

\[
\frac{a\sqrt{C_{11}}}{C_{12}} - 1 = b\sqrt{C_{11}}\frac{C_{13}}{C_{13}} - 1 = c\sqrt{C_{22}}\frac{C_{23}}{C_{23}} - 1 = 0
\]

(21)

which can be further simplified as:

\[
\left( \frac{a\sqrt{C_{11}}}{C_{12}} - 1 \right)^2 + \left( \frac{b\sqrt{C_{11}}}{C_{13}} - 1 \right)^2 + \left( \frac{c\sqrt{C_{22}}}{C_{23}} - 1 \right)^2 = 0
\]

(22)

Finally, since \( C_{ii} \geq 0 \) \( (i = 1, 2, 3, 4, 5, 6) \), we can rewrite the equation \( C_{44} = C_{55} = C_{66} = 0 \) in the Eq. (6) as the following form:

\[
\frac{C_{44} + C_{55} + C_{66}}{C_{11} + C_{22} + C_{33}} = 0
\]

(23)

Therefore, the sum of left-side terms in Eqs. (22) and (23) must also be zero. Then a general mathematical optimization model can be defined as follows:

\[
\text{Find } \mathbf{\rho} = [\rho_1 \ \rho_2 \ \cdots \ \rho_{n_{\text{var}}} - 1 \ \rho_{n_{\text{var}}}]^T
\]

(24)
Min : $f(\rho) = \frac{(a \sqrt{C_{11}^{H}(\rho)C_{22}^{H}(\rho)}}{C_{12}^{H}(\rho)} - 1)^2 + \frac{(b \sqrt{C_{11}^{H}(\rho)C_{33}^{H}(\rho)}}{C_{13}^{H}(\rho)} - 1)^2$

$$+ \frac{(c \sqrt{C_{22}^{H}(\rho)C_{33}^{H}(\rho)}}{C_{23}^{H}(\rho)} - 1)^2 + C_{44}^{H}(\rho) + C_{55}^{H}(\rho) + C_{66}^{H}(\rho)$$

subject to:

$$C_{ij}^{H}(\rho) = 0, i = 1, 2, 3, j = 4, 5, 6$$

$$C_{45}^{H}(\rho) = C_{46}^{H}(\rho) = C_{65}^{H}(\rho) = 0$$

where $C^{H}$ is the effective elasticity matrix of the ground structure estimated by the numerical homogenization method considering the periodic boundary condition [32]. $\rho$ is a vector of binary variables representing whether each bar in the ground structure is active or not, $n_{\text{bar}}$ is the number of bars in the ground structure. It is noted that a choice of $a, b$ and $c$ that belongs to the four cases in Eq. (14) should be determined in advance. We would emphasize that the dominator $C_{11}^{H}(\rho) + C_{22}^{H}(\rho) + C_{33}^{H}(\rho)$ is not necessary in the objective function but it is used to normalize the last term to enhance the optimization performance.

The constraints in Eq. (24) are to ensure that the optimized lattices have at least orthotropic symmetry. When the objective function value approaches to zero (globally minimum value), the necessary and sufficient condition required for elasticity matrix of pentamode metamaterials with at least orthotropic symmetry will be satisfied. It is noted that for such an inverse design problem, multiple solutions may exist.

As mentioned above, the design variables are 0 and 1 logical variables representing which bars are active. However, it does not mean

---

**Fig. 2.** Mesh nodes and the corresponding ground structure.

**Fig. 3.** Different groups of bars.
that inactive bars are not included in finite element analyses of the numerical homogenization. That is because the total stiffness matrix of a mechanism-type pentamode lattice that only consists of active bars is singular in numerical. Therefore, inactive bars are assigned with relatively small axial stiffness and then included in the numerical homogenization. This can prevent the total stiffness matrix from being singular but the effect to the value of the effective elasticity matrix is small and acceptable.

3.2. Optimization solver

Recently, Wang et al. [31] has studied the design of materials with prescribed nonlinear properties using the ground structure method, which uses artificial densities of each bar as continuous design variables and the mathematical programming method to solve the problem. In this paper, we will also use the ground structure method to design pentamode metamaterials, but the genetic algorithm [33] is adopted to solve this discrete optimization problem with binary variables.

---

**Fig. 4.** Intersection and overlap of two bars.

**Fig. 5.** Shortest line between two lines in three dimensions.

**Fig. 6.** Flowchart of the detection method for intersection and overlap of bars.

**Fig. 7.** Overlapping bars in the ground structure.
A genetic algorithm is in general known as a global optimization method based on natural selection. It randomly generates an initial population. During the iteration, individuals with better fitness values in the current population will be selected as parents. Then three types of children are produced from parents to form the next generation. Elite children are individuals with best fitness values, crossover children are generated by combining pairs of parents, and mutation children are generated by making random changes to individual parents [33]. In the numerical implementation, we use the built-in Matlab function for the genetic algorithm.

The genetic algorithm is not often used to solve topology optimization problems for no matter continuum or discrete structures, although it is a heuristic optimization method with global searching capability. The first main reason is that there are usually thousands or even millions of continuous design variables in topology optimization problems. It is difficult for genetic algorithms to find a
solution for large-scale optimization problems with continuous variables. The second reason is that the calculation of the objective and constraint functions with large-scale finite elements is computationally expensive. Unfortunately, thousands of times of evaluation of candidate solutions is common for the genetic algorithm, while mathematical programming methods using sensitivity information usually need up to hundreds of times of finite element analyses.

However, the ground structure used in this paper is a very small-scale truss model with only hundreds of binary design variables. It is also cheap in computation to run finite element analyses in parallel. Therefore, instead of using mathematical programming methods, the genetic algorithm is used in this paper as the optimization solver to find the global optimal solution, since the discrete optimization problem here is relatively small scale and cheap in computation.

In this work, the max number of optimization iterations is set to 200, and the population size is 1000. Calculation of the objective function runs in parallel using a 6-core Intel i7-8750H CPU. For the maximum 0.2 million times of finite element analyses and numerical homogenization evaluations, it only costs around 25 min when using the ground structure described in Section 3.3.

### 3.3. Generation of the ground structure

For a given set of mesh nodes, the easiest way to generate a ground structure is just linking every two nodes. The number of bars for such a fully connected ground structure is equal to \((n_{\text{node}}^2 - n_{\text{node}})/2\), where \(n_{\text{node}}\) is the number of nodes. Zegard and Paulino [34] proposed a method to generate ground structures in arbitrary three-dimensional domains with control in the level of redundancy or inter-connectedness of ground structures. However, it cannot guarantee that optimized lattices have at least orthotropic material symmetry. Therefore, a new ground structure with geometrically orthotropic symmetry is proposed in this paper as the optimization solver to find the global optimal solution, since the discrete optimization problem here is relatively small scale and cheap in computation.

We suppose there are \(5 \times 5 \times 5\) Cartesian mesh nodes centered at the origin and aligned with coordinate axes as shown in Fig. 2a, and then the corresponding ground structure with geometrically orthotropic symmetry will be as shown in Fig. 2b. Due to the geometrically orthotropic symmetry, the design variables are changed from \(\rho\) to \(\tilde{\rho}\) as defined in Eq. (20), which is still a vector of binary design variables.

\[
\tilde{\rho} = \left[ \tilde{\rho}_1 \quad \tilde{\rho}_2 \quad \cdots \quad \tilde{\rho}_{n_{\text{des}}} \right]
\]

where \(n_{\text{des}}\) is the number of design variables. For the ground structure in Fig. 2b, the numbers of bars and design variables are 2544 and 405 respectively, while for a fully connected ground structure both the bar number and design variables will be as large as 7750.

The bars in the ground structure are divided into five groups as shown in Fig. 3. The bars of the first group are collinear with one coordinate axis and symmetric about one coordinate plane. Each of these bars has no mirrored copies in the ground structure as shown in Fig. 3a. Therefore, 6 design variables of this group correspond to 6 bars. The second group consists of two types of bars. One type is collinear with one coordinate axis and on the side of one coordinate plane. The other type is coplanar with one coordinate plane, parallel but not collinear with one coordinate axis and then symmetric about another coordinate plane. Each of these bars has another mirrored copy in the ground structure as shown in Fig. 3b. Therefore, 33 design variables of this group correspond to 66 bars. The bars of the third group are coplanar with one coordinate plane and on the side of other coordinate planes. Each of these bars has other three mirrored copies in the ground structure as shown in Fig. 3c. Therefore, 90 design variables of this group correspond to 360 bars. The bars of the fourth group are symmetric about one coordinate plane and parallel but not coplanar with other coordinate planes. Each of these bars has other three mirrored copies in the ground structure as shown in Fig. 3d. Therefore, 24 design variables of this group correspond to 96 bars. Finally, the fifth group is obtained by linking every two nodes in the same octant and then subtracting bars that already belong to the aforementioned four groups. Each of these bars has other seven mirrored copies in the ground structure as shown in Fig. 3e. Therefore, 252 design variables of this group correspond to 2016 bars.

For the educational purpose, we provide two Matlab scripts online for free download and use at https://github.com/appreciator/Ground-Structure. One script can be used to generate ground structures with geometrically orthotropic symmetry as introduced above. The other script can determine which bars are active according to the given design variables. The numbers of Cartesian mesh nodes are chosen as user-input values, and therefore the reader can obtain much more complex ground structures. It is noted that the lattices do not always have to be geometrically orthotropic symmetric. Therefore, other potential pentamode lattices without geometrically orthotropic symmetry, e.g., the conventional diamond-type pentamode lattice, cannot be discovered by using the ground structure proposed in this paper.

### 3.4. Geometric constraints

Definitions of intersection and overlap of bars are illustrated in Fig. 4.

Geometric constraints on intersection and overlap of bars in ground structure methods have already been introduced for macro-scale structures [35,36], but not yet been introduced for lattice designs [29–31]. In engineering, intersectional points have no physical meaning except in the form of hinge points [36]. Optimization solutions with existence of intersection or overlap of bars are unrealistic designs [36]. Such impractical topologies should be avoided for optimized lattices. Therefore, constraints on intersection and overlap of bars should be imposed on optimization design of pentamode metamaterials. Cui et al. [36]
provided a mathematical recognition method for intersection and overlap of bars in three-dimensional ground structures. However, it is not computationally efficient, e.g. linear equations should be solved for each two bars. Based on calculating the shortest line between two lines in three dimensions, we propose a new mathematical recognition method in this paper.

As shown in Fig. 5, the lines AB and CD do not intersect at a point, and the line EF is the shortest line between them. Coordinates of the points E and F are defined as:

\[
\begin{align*}
    x_E &= x_A + \mu_E (x_B - x_A) \\
    x_F &= x_C + \mu_F (x_D - x_C)
\end{align*}
\]
The values of $\mu_k$ and $\mu_k$ range from negative to positive infinity. $\mu_k$ can be calculated by the following formula, while $\mu_k$ can be calculated by substituting subscripts:

$$\mu_k = \frac{d_{ABCD}d_{BCDA} - d_{ABDC}d_{CDAB}}{d_{ABBA}d_{BCDC} - d_{BCBD}d_{CDAB}}$$  \hspace{1cm} (27)$$

where

$$d_{MNOP} = (x_M - x_N)(x_O - x_P) + (y_M - y_N)(y_O - y_P) + (z_M - z_N)(z_O - z_P)$$  \hspace{1cm} (28)$$

when AB and CD intersect, E and F are coincident and the values of $\mu_k$ and $\mu_k$ are between 0 and 1. when AB and CD are parallel, the dominator in Eq. (27) is zero. Details of mathematical derivation can be referred to [37].

Under the assumption that AB and CD are parallel, if points A, B and C are collinear, lines AB and CD will be collinear. For three points to be collinear, the following equation should be satisfied:

$$\begin{align*}
(x_c - x_a)(y_b - y_a) &= (x_c - x_b)(y_a - y_b) \\
(x_c - x_a)(z_b - z_a) &= (x_c - x_b)(z_a - z_b) \\
(y_c - y_a)(z_b - z_a) &= (y_c - y_b)(z_a - z_b)
\end{align*}$$  \hspace{1cm} (29)$$

For two lines to be coplanar, the following equation should be satisfied:

$$\vec{AC} \cdot (\vec{AB} \times \vec{CD}) = 0$$  \hspace{1cm} (30)$$

The flowchart about how to detect intersection and overlap of each two bars is given in Fig. 6.

Since genetic algorithms cannot handle nonlinear constraints like mathematical programming methods, geometric constraints on intersection and overlap are added as a penalty term into the original objective function in Eq. (24). The modified objective function is defined as:

$$f(\hat{\rho}) = f(\rho) + w \frac{n_{\text{ins}}(\hat{\rho}) + n_{\text{ovl}}(\hat{\rho})}{n_{\text{geo}}}$$  \hspace{1cm} (31)$$

where $n_{\text{geo}}$ is the total number of intersection and overlap of the fully active ground structure, $n_{\text{ins}}$ is the number of intersection of the current design, $n_{\text{ovl}}$ is the number of overlap of the current design, and $w$ is a weighting factor.

For a design without any intersection or overlap of bars, the penalty value becomes zero, and then the modified objective function is the same as the original one. Normalized by the dominator $n_{\text{geo}}$, the penalty value will not be larger than $w$. Since the value of $f(\hat{\rho})$ approaches to zero during the optimization iteration, the value of $w$ can absolutely be a small number but still relatively large enough compared with zero. Therefore, we choose $w = 0.001$ in this work.

It is noted that ground structures generated by the method in [34] do not have a single bar connecting the same nodes with other two bars as shown in Fig. 7. However, these two cases of bars may have different influence on pentamode behavior of lattices, and we cannot determine which case should be adopted for different local locations in the ground structure in advance. Therefore, these two cases of bars both initially exist in the ground structure described in Section 3.3. However, we emphasize that since geometric constraints have been imposed as a penalty term in the objective function, such an overlapping case will not exist in the final optimized designs.

### 4. Numerical results

Twenty-four new pentamode lattices without any intersection or overlap of bars will be provided here to demonstrate the effectiveness of the proposed design method, including isotropic, transverse isotropic and orthotropic ones. In this section, we will give results for numerical verification of non-isotropic pentamode lattices. We will further compare the static mechanical performance of two lattices, respectively, assembled by new isotropic pentamode lattices and the conventional diamond-type isotropic lattices. Moreover, we will study on how to obtain pentamode lattices with different relative densities from the optimization results.

#### 4.1. New pentamode lattices

As shown in Fig. 2b, the ground structure is generated by $5 \times 5 \times 5$ mesh nodes with 2544 bars and 405 design variables. The side length of its bounding box is 1 mm. Truss elements are used in finite element analyses. The Young’s modulus is 1.138e5 MPa. Constant diameters of active and inactive bars are 0.02 mm and 2.0e-6 mm respectively. We define $\lambda_{\text{max},1}$ as the maximum eigenvalue of the effective elasticity matrix of a lattice, $\lambda_{\text{max},2}$ as the second maximum eigenvalue, and $\lambda_{g}$ as the ratio between them. For perfect pentamode metamaterials, $\lambda_{g}$ should approach infinity. In the following, three tables are given in this section, and note that the unit of elastic constants is MPa. A smaller scale of $2 \times 2 \times 2$ periodic array is given on the right side together with the lattice on the left side in each sub-figure. It is noted that each periodic array visualized here is smaller scale than the lattice.

Eight isotropic pentamode lattices are shown in Fig. 8. The corresponding effective elasticity matrices and eigenvalue ratios are listed in Table 1.

Eight transverse isotropic pentamode lattices are shown in Fig. 9. The corresponding effective elasticity matrices and eigenvalue ratios are listed in Table 2.

Eight orthotropic pentamode lattices are given in Fig. 10. The corresponding effective elasticity matrices and eigenvalue ratios are listed in Table 3.
From the above three tables, we can see that the homogenized effective elasticity matrices of these twenty-four lattices all satisfy the requirement of pentamode metamaterials.

4.2. Stress modes of non-isotropic pentamode lattices

As mentioned previously, pentamode metamaterials can bear only single mode of stress, which is proportional to the eigenvector corresponding to the non-zero eigenvalue of the elasticity matrix [1]. Here, we name them as stress modes. For non-isotropic pentamode lattices obtained by topology optimization in this paper, their feature is that they can bear load cases proportional to the Eq. (16). We will give linear static analysis results of lattices assembled by non-isotropic pentamode lattices to verify that they are stiffer when subjected to the load cases. The lattices Trans-a and Ortho-a are chosen as examples.

Fig. 10. Orthotropic pentamode lattices.
The loads and boundary conditions are given in Fig. 11. The blue cube represents the bounding box of the lattice structure assembled by $6 \times 6 \times 6$ periodic lattices, measuring 6 mm on one side. For each pair of the opposite faces, the equal magnitude but opposite pressure is uniformly applied. The magnitudes of the resultant forces along each axis are $F_x$, $F_y$ and $F_z$. Due to the symmetry, only one-eighth of the model (i.e., $3 \times 3 \times 3$ lattices) is used in finite element analyses with symmetric boundary conditions. We name the structure assembled by transverse isotropic lattices as the lattice I and the structure assembled by orthotropic lattices as the lattice II. For all the lattices, the diameters of uniform cylinder bars are 0.02 mm. These solid lattices are meshed with linear tetrahedral elements, and the global element seed size is 0.004 mm. The Young’s modulus for the base material Ti6Al4V is $1.138 \times 10^5$ MPa, and the Poisson’s ratio is 0.342.

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Six typical load cases applied to each lattice structure are listed in Table 4. The fifth and sixth cases are proportional to the load cases of the transverse isotropic and orthotropic lattices, respectively. The load cases are calculated by the eigenvector of the homogenized effective elasticity matrices of the solid lattices. It is noted that for all these load cases, the vector sum of three forces are the same as $1.73205 \times 10^{-2}$ N.

The results of linear static finite element analyses using ABAQUS are given below. From Fig. 12 and Table 5, we can find that for the lattice I, both the displacement magnitude and the total strain energy in the fifth load case are the smallest. From Fig. 13 and Table 5, we can also find that for the lattice II, both the displacement magnitude and the total strain energy in the sixth load case are the smallest. We emphasize that the total strain energy ratios of the load case to other load cases are considerably small. In one word, a lattice assembled by non-isotropic pentamode lattices is much stiffer when bearing the load case.

### 4.3. Comparison with conventional diamond-type pentamode lattice

Here, we will take the new isotropic pentamode lattice Iso-f as an example to compare the static mechanical performance of the new lattices with the conventional diamond-type isotropic pentamode lattice. Like the models in Section 4.2, each lattice used in finite element analyses consists of $3 \times 3 \times 3$ periodic lattices, and symmetric boundary conditions are applied. The values of $F_x$, $F_y$ and $F_z$ are all set to $0.01$ N. We name the lattice structure assembled by new isotropic lattices as the lattice III, and the lattice structure assembled by diamond-type lattices as the lattice IV. For the lattice III, the diameters of uniform cylinder bars are 0.02 mm. For the lattice IV, the diameters of double-cone bars are $d = 0.02$ mm and $D = 0.0241$ mm. It is noted that the two lattices have the same material volume ($0.071$ mm$^3$). The mesh and base material properties are the same as models given in Section 4.2.

#### Table 3
Effective properties of orthotropic pentamode lattices.

<table>
<thead>
<tr>
<th></th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>d</th>
<th>e</th>
<th>f</th>
<th>g</th>
<th>h</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{11}$</td>
<td>5.677</td>
<td>7.323</td>
<td>38.291</td>
<td>92.377</td>
<td>77.083</td>
<td>11.046</td>
<td>27.313</td>
<td>90.835</td>
</tr>
<tr>
<td>$C_{12}$</td>
<td>22.709</td>
<td>29.291</td>
<td>86.156</td>
<td>10.260</td>
<td>34.259</td>
<td>99.413</td>
<td>109.253</td>
<td>10.093</td>
</tr>
<tr>
<td>$C_{22}$</td>
<td>51.096</td>
<td>65.905</td>
<td>9.573</td>
<td>41.039</td>
<td>8.565</td>
<td>44.183</td>
<td>6.828</td>
<td>40.371</td>
</tr>
<tr>
<td>$C_{33}$</td>
<td>11.355</td>
<td>14.646</td>
<td>57.437</td>
<td>30.779</td>
<td>51.389</td>
<td>33.138</td>
<td>54.626</td>
<td>30.278</td>
</tr>
<tr>
<td>$C_{44}$</td>
<td>0.173</td>
<td>0.219</td>
<td>0.191</td>
<td>0.615</td>
<td>0.257</td>
<td>0.221</td>
<td>0.137</td>
<td>0.606</td>
</tr>
</tbody>
</table>

#### Table 4
Load cases for the lattices.

<table>
<thead>
<tr>
<th>Case</th>
<th>Case 2</th>
<th>Case 3</th>
<th>Case 4</th>
<th>Case 5</th>
<th>Case 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F_x/N$</td>
<td>1.73205e-2</td>
<td>0</td>
<td>0</td>
<td>1.0e-2</td>
<td>1.15474e-2</td>
</tr>
<tr>
<td>$F_y/N$</td>
<td>0</td>
<td>1.73205e-2</td>
<td>0</td>
<td>1.0e-2</td>
<td>1.15474e-2</td>
</tr>
<tr>
<td>$F_z/N$</td>
<td>0</td>
<td>0</td>
<td>1.73205e-2</td>
<td>1.0e-2</td>
<td>5.77213e-3</td>
</tr>
</tbody>
</table>

Fig. 11. Loads and boundary conditions.
The linear static analysis results are given in Figs. 14 and 15. For the lattice III, over 90% of the von Mises stresses of Gauss integration points are between 1.2 MPa and 1.3 MPa, and the ratio of the maximum value to the minimum value is not over 4. The stress distribution in the lattice III is relatively uniform. For the lattice IV, we can see that it suffers from the stress concentration. The maximum von Mises stress of the lattice IV (146.633 MPa) is much higher than that of the lattice III (2.135 MPa).

The linear buckling analysis results are given in Fig. 16. The lowest buckling load of the lattice III ($F_x = F_y = F_z = 0.253$ N) is slightly higher than that of the lattice IV ($F_x = F_y = F_z = 0.241$ N). We can see that the first buckling modes of the two lattices all show overall buckling.

From the concept of linear static analysis, we can know that when the load is close to $F_x = F_y = F_z = 0.253$ N, the maximum von Mises stress of the lattice III is only 54 MPa. However, for the lattice IV, even when the load is close to $F_x = F_y = F_z = 0.253$ N, the maximum von Mises stress of the lattice IV is much higher than that of the lattice III.

### Table 5

<table>
<thead>
<tr>
<th>Case</th>
<th>Case 2</th>
<th>Case 3</th>
<th>Case 4</th>
<th>Case 5</th>
<th>Case 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice I</td>
<td>1.51e-4</td>
<td>1.34e-4</td>
<td>1.14e-3</td>
<td>9.61e-5</td>
<td>8.77e-7</td>
</tr>
<tr>
<td>Lattice II</td>
<td>5.82e-4</td>
<td>4.80e-5</td>
<td>1.18e-4</td>
<td>9.93e-5</td>
<td>2.25e-4</td>
</tr>
</tbody>
</table>

Fig. 12. Displacement results of the lattice I (Unit: mm).

Fig. 13. Displacement results of the lattice II (Unit: mm).
the load is two-thirds of its lowest buckling load (i.e. \( F_x = F_y = F_z = 0.1607 \text{ N} \)), the maximum von Mises stress theoretically reaches about 2356 MPa and already exceeds the ultimate bearing strength (1860 MPa) of the base material Ti6Al4V. Therefore, no matter the strength or buckling, the lattice III can bear much higher hydrostatic stress than the lattice IV.

### 4.4. Pentamode lattices with different relative densities

The proposed design method in this work gives a topologically optimal layout of the solid bars in the space. Based on the optimized skeleton, pentamode lattices with different relative densities can be obtained by changing the geometric dimensions and shapes of the bars. For example, we can introduce the double-cone bars in [3] to replace the uniform cross-section bars, and then change the mid-span diameters \( D \) to obtain different relative densities. We emphasize here that other types of structural members rather than double-cone bars can be used to form the pentamode lattices based on the topologically optimized layout.

Take the optimized skeleton shown in Fig. 8f as the example. For the lattice in Fig. 17a, the diameter of uniform cylinder bars is 0.02 mm. Based on the same skeleton, a pentamode lattice using double-cone bars is generated as shown in Fig. 17b, of which the diameters are \( d = 0.02 \text{ mm} \) and \( D = 0.06 \text{ mm} \). The mesh setting and base material properties are the same as models in Section 4.2.

The effective elasticity matrices, eigenvalue ratios and relative densities \( \rho_R \) are listed in Table 6, as below. The unit of elastic constants is MPa. From Table 6, we can find that all eigenvalue ratios are relatively large enough to consider these lattices to be pentamode, while the lattices are based on the same skeleton but have different relative densities (0.256\% and 1.143\%). It is noted that the homogenized shear moduli of the solid structures do not approach to zero, but they are still relatively small enough to allow reasonable pentamode properties.

A micro-lattice (Fig. 18) with \( 2 \times 2 \times 2 \) lattices as given in Fig. 17b is prototyped using the Digital Light Processing (DLP) technique, with Octave Light R1 machine using a rubber-like material (TangoGray FLX950), as shown in Fig. 19.

### 5. Conclusions

This work has derived the necessary and sufficient condition required for elasticity constants of pentamode metamaterials with at least orthotropic symmetry. We found that a large ratio of the bulk modulus to the shear modulus is no more a sufficient condition for
Fig. 16. First buckling modes of the lattices.

Fig. 17. Mesh models of pentamode lattices using tetrahedral elements.
non-isotropic pentamode metamaterials. A ground structure method with the genetic algorithm is then proposed to conduct topology optimization of pentamode metamaterials with at least orthotropic symmetry. Geometric constraints on intersection and overlap of bars are applied to the lattice with a new efficient detection method to obtain realistic designs. Twenty-four new pentamode lattices without intersection or overlap of bars are discovered, including isotropic, transverse isotropic and orthotropic ones. The optimization results have demonstrated the effectiveness and efficiency of the proposed design method. The further analyses have verified that lattices assembled by non-isotropic pentamode lattices are much stiffer when subjected to their bearable load cases. From the comparative analysis results, we can see that one isotropic pentamode lattice obtained by topology optimization can form lattices to bear much higher hydrostatic stress than the conventional diamond-type pentamode lattice. Moreover, we propose that based on the optimized skeleton, pentamode lattices with different relative densities can be obtained just by changing the geometric dimensions and shapes of the bars.

In the future, we will further derive the necessary and sufficient condition required for elasticity constants of fully anisotropic pentamode lattices, and modify the mathematical optimization model based on the derived condition. Then the topology optimization design framework proposed in this paper can also be used to find new fully anisotropic pentamode lattices with minor modifications. Moreover, potential applications of the new pentamode lattices on cloaking devices will also be our next study.

Authors’ contribution

Zuyu Li: Writing - original draft; Formal analysis; Investigation; Methodology.
Zhen Luo: Conceptualization; Funding acquisition; Project administration; Supervision; Writing - review & editing.

<table>
<thead>
<tr>
<th>Table 6</th>
<th>Effective properties of pentamode lattices using solid elements.</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>b</td>
</tr>
<tr>
<td>$C_{11}$</td>
<td>33.969 108.438</td>
</tr>
<tr>
<td>$C_{22}$</td>
<td>33.970 108.453</td>
</tr>
<tr>
<td>$C_{33}$</td>
<td>33.970 108.453</td>
</tr>
<tr>
<td>$C_{12}$</td>
<td>33.795 107.649</td>
</tr>
<tr>
<td>$C_{13}$</td>
<td>33.795 107.648</td>
</tr>
<tr>
<td>$C_{23}$</td>
<td>33.795 107.656</td>
</tr>
<tr>
<td>$C_{44}$</td>
<td>0.091 0.420</td>
</tr>
<tr>
<td>$C_{55}$</td>
<td>0.091 0.420</td>
</tr>
<tr>
<td>$C_{66}$</td>
<td>0.091 0.420</td>
</tr>
<tr>
<td>$\lambda_{\text{max},1}$</td>
<td>101.561 323.750</td>
</tr>
<tr>
<td>$\lambda_{\text{max},2}$</td>
<td>0.175 0.797</td>
</tr>
<tr>
<td>$\lambda_R$</td>
<td>581.864 406.004</td>
</tr>
<tr>
<td>$\rho_R$ (%)</td>
<td>0.256 1.143</td>
</tr>
</tbody>
</table>

Fig. 18. Periodic arrays of the pentamode lattices.

(a) Additively manufactured specimen (b) Microscopic photo

Fig. 19. An additively manufactured micro-lattice with $2 \times 2 \times 2$ lattices.
Lai-Chang Zhang: Validation; Visualization; Resources.
Chun-Hui Wang: Data curation; Formal analysis; Investigation.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper. The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

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