Topological design of microstructures of cellular material using energy-based homogenization method

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Abstract: With the fact that the microstructure of light-weight cellular materials having a significant impact on its macro performance, the material or structure with special macroscopic properties can be obtained through the topological design of the microstructure of cellular material. Based on this idea, this paper focuses on determining the optimal material layout in the periodic microstructural unit cell. The effective elastic properties of the periodic microstructure are obtained by using an efficient energy-based homogenization method. The optimization model is formulated as finding a microstructural topology with extreme properties or desired properties under the constraints of a prescribed volume fractions based on topology optimization technique. In this framework, the SIMP interpolation combined with OC algorithm is utilized to solve the problem. Several typical numerical examples are presented to demonstrate the favorable characteristics of the proposed method in the optimization design of material microstructures. Some interesting topological configuration have been found for guiding the cellular material design.

Keyword: Topology optimization；energy-based homogenization；cellular material；microstructure design；SIMP interpolation

1. Introduction

The development of modern engineering technology has increasingly high requirements to the performance of materials, and new materials and structures with special mechanical properties are needed. Light-weight cellular materials have been widely concerned due to the various advanced physical，mechanical and thermal properties far more beyond solid materials[1]. They are usually characterized by assemblies of a number of periodical microstructures, consisting of conventional materials, such as metals or plastics. Thus the layout of the unit cell of microstructure has an utmost impact on the properties of cellular materials. Therefore, it is of great interest to apply topology optimization methods to achieve the optimal material layout of the unit cell of periodic microstructure, which has the desired properties or even extreme properties[2].

In the last decades, topology optimization has been expanding as a powerful computational design tool for structures and materials both in academic research and industrial applications[3]. Essentially, topology optimization is a numerical iterative method that distributes a given amount of material inside a prescribed design domain to seek the optimal material layout, such that the objective function is optimized subject to a set of constraints[2]. So far, various methods have been developed for topology optimization, e.g. the homogenization method[4,5], the evolutionary structural optimization method(ESO)[6,7]and bi-directional evolutionary structural optimization (BESO)[8-9], the element density SIMP method[10,11], the nodal density SIMP method[12,13], and the level set based method(LSM)[14,15]. Amongst a number of applications of topology optimization, one of the most promising applications may be the optimization design of material microstructures [2].

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For instance, Sigmund[16, 17]firstly employed the topology optimization method to design periodic microstructures with prescribed properties based on the inverse homogenization method. Since then, topology optimization has showcased the potential in the design of various materials. Such as, Gibiansky and Neves et al[18,19]designed multiphase composites with extreme elastic properties subject to the constraint of volume fraction of materials. Sigmund et al [20,21]obtained the composites with zero or negative thermal expansion coefficients using a numerical topology optimization method. Huang and Andreassen et al[22,23]designed the periodic composite microstructure with optimal viscoelastic characteristics. Grimberg and Zhou et al. [24,25]have extended a level set procedure to design the electromagnetic meta-materials. Luo and Andreassen et al[2,26]proposed a new topological optimization method to design a type of mechanical metamaterials with negative Poisson's(auxetic materials). Wang[27]obtained the material microstructures with prescribed nonlinear properties using topology optimization under finite deformation. Zhou and Li[28,29]have investigated the computational design of composite microstructural for extremal conductivity property or graded mechanical property using the SIMP method.

However, the method mentioned above are mainly focused on obtaining the effective properties of the periodic microstructures through the numerical homogenization method, and then the optimization problem for seeking the optimal microstructure of the unit cell with the different properties was realized. Compared with the homogenization method, the energy-based homogenization method is of higher computational efficiency and more simplified programming. Zhang et al. [30-31] and Xia et al. [32] have investigated the design of material microstructures with extreme elastic properties using energy-based homogenization method, but for the design of material microstructures with prescribed properties haven't too much involved. More importantly, because there is no unique solution for material design, the optimization iterative algorithm is hard to converge, and the optimization parameters are difficult to be selected in the design of material microstructures. All of the mentioned problems above have not been discussed too much in these literatures.

In this paper, the effective elastic properties of the periodic microstructure are evaluated by using an efficient energy-based homogenization method. The optimization problem is formulated as achieving an optimal microstructure with extreme properties or desired properties under the constraint of a prescribed volume fractions based on topology optimization technique. The SIMP interpolation combined with OC algorithm is utilized to solve the problem. What's more, at the beginning of the optimization iteration, an appropriate number of holes are to put in the initial configuration, which could increase the inhomogeneity of the design domain and have certain guidance on the optimal microstructure configuration at the same time, so as to solve the problem of multiple solutions during the material designing procedure. Thus the oscillation of the objective function could be avoided in the iterative process, and the sensitivity of optimization algorithm on the optimization parameters could be reduced, and the computational efficiency would be improved to a great extent.

2. The energy-based homogenization and sensitivity analysis

2.1 The equivalent method of effective elastic properties based on the energy-based homogenization

Based on the homogenization theory, the effective elastic tensor D_{ijkl}^{H} of the periodic material microstructures can be formulated as the following symmetrical form[16]

$$D_{ijkl}^{H} = \frac{1}{|Y|}\int_{Y}\left(\varepsilon_{pq}^{0(ij)} - \varepsilon_{pq}^{*(ij)}\right)D_{pqrs}\left(\varepsilon_{rs}^{0(kl)} - \varepsilon_{rs}^{*(kl)}\right)dY \tag{1}$$

Where ε_{pq}^{0} is the macroscopic strain fields, consisting of three components (e.g. horizontal unit strain, vertical unit strain and shear unit strain), while ε^{*}_{pq} is the locally varying strain fields.

In order to utilize the more mature topology optimization technology in the field of structural optimization, (1) can be written in the form of an equivalent form (2) based on the element mutual energies[16]

$$D^H_{ijkl} = \frac{1}{|Y|}\int_Y D_{pqrs}\varepsilon^{A(ij)}_{pq}\varepsilon^{A(kl)}_{rs}dY \tag{2}$$

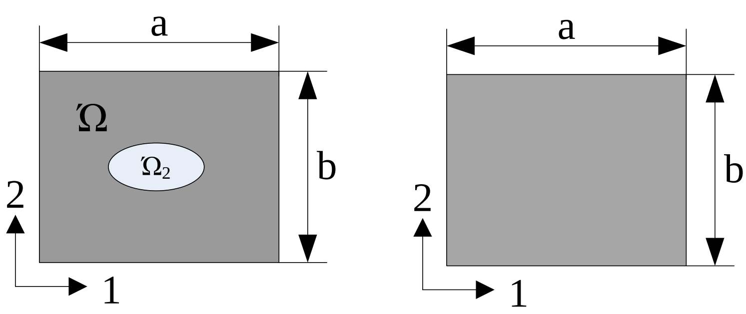
In finite element analysis, the unit cell of microstructure is discretized into N finite elements, and（2）is written as following approximately

$$D^H_{ijkl} = \frac{1}{|Y|}\sum_{e=1}^{N}\left(u_e^{A(ij)}\right)^T k_e u_e^{A(kl)} = \frac{1}{|Y|}\sum_{e=1}^{N} q_e^{(ijkl)} \tag{3}$$

Where $q_e^{(ijkl)}$ is the element mutual energy, and $u_e^{A(kl)}$ are the element displacement fields corresponding to the macroscopic strain fields $\varepsilon^{0(kl)}$, and k_e is the element stiffness matrix. In the two-dimensional plane stress problem, we note that $11 \to 1$, $22 \to 2$, $12 \to 3$, allowing to write (3) in an expanded form (we assume the materials are isotropic)

$$\begin{bmatrix} D^H_{11} & D^H_{12} & 0 \\ D^H_{12} & D^H_{22} & 0 \\ 0 & 0 & D^H_{33} \end{bmatrix} = \begin{bmatrix} Q_{11} & Q_{12} & 0 \\ Q_{12} & Q_{22} & 0 \\ 0 & 0 & Q_{33} \end{bmatrix} \tag{4}$$

Where the terms $Q_{ij} = \frac{1}{|Y|}\sum_{e=1}^{N} q_e^{(ij)}$ 。



(a) (b)

Fig.1 Homogenization of 2D microstructure.

(a) microstructure, (b) equivalent homogenized medium.

The microscopic inhomogeneous structure namely the periodic microstructure shown in Fig. 1(a) can be replaced by an equivalent homogeneous medium with the same volume at the macroscopic level as shown in Fig. 1(b).

The stress and the strain tensors of the homogeneous medium and the average stress and strain of the microstructure satisfy the following conditions[31]

$$\bar{\sigma} = \frac{1}{V}\int_\Omega \sigma d\Omega\, , \quad \bar{\varepsilon} = \frac{1}{V}\int_\Omega \varepsilon d\Omega \tag{5}$$

The stress and the strain tensors of the homogeneous medium also follow the Hooke's law

$$\bar{\sigma} = D^H \bar{\varepsilon} \tag{6}$$

Where D^H is the effective elastic tensor of the material microstructure.

According to (4),（6）can be further formulated as

$$\begin{bmatrix} \overline{\sigma}_{11} \\ \overline{\sigma}_{22} \\ \overline{\sigma}_{12} \end{bmatrix} = \begin{bmatrix} D^H_{1111} & D^H_{1122} & 0 \\ D^H_{1122} & D^H_{2222} & 0 \\ 0 & 0 & D^H_{1122} \end{bmatrix} \begin{bmatrix} \overline{\varepsilon}_{11} \\ \overline{\varepsilon}_{22} \\ \overline{\varepsilon}_{12} \end{bmatrix} \tag{7}$$

Where $\overline{\sigma}_{11}$, $\overline{\sigma}_{22}$ denotes the averaged stress in the horizontal and vertical direction respectively, and $\overline{\varepsilon}_{11}$, $\overline{\varepsilon}_{22}$ denotes the averaged strain in corresponding two directions, and $\overline{\sigma}_{12}$, $\overline{\varepsilon}_{12}$ denotes the averaged shear stress and strain.

Besides, regardless of the influence of temperature, the strain energies stored in microstructure and the homogeneous medium has to be equal

$$\begin{aligned} & Q(\varepsilon) = Q(\overline{\varepsilon}) \\ & = \frac{1}{V}\int_{\Omega}(\sigma_{11}\varepsilon_{11} + \sigma_{22}\varepsilon_{22} + \sigma_{12}\varepsilon_{12})d\Omega \\ & = \frac{1}{2}(\overline{\sigma}_{11}\overline{\varepsilon}_{11} + \overline{\sigma}_{22}\overline{\varepsilon}_{22} + \overline{\sigma}_{12}\overline{\varepsilon}_{12}) \end{aligned} \tag{8}$$

According to Eqs.(7) and (8),the corresponding unit strain energy of the microstructure can be calculated under the specific boundary conditions, such as specific strain fields and periodic boundary conditions. And then, the relationship between the effective elastic modulus and the corresponding unit strain energy of the microstructure can be derived, thus the energy expression of the effective elastic modulus of the microstructure can be obtained. As shown in Fig. 1, the unit volume microstructure under plane stress state is set to be an example (a and b is selected as a=b=1), the effective elastic properties can be calculated by the prescribed displacement boundary conditions as shown in Table 1 (set u=v=a/2=0.5 in the Table 1).

Table 1 Prescribed boundary conditions and corresponding strain energies of microstructures

Boundary condition	Strain energies of microstructure
Horizontal strain $\overline{\varepsilon}^{(1)} = [1 \quad 0 \quad 0]^T$	$Q^{(1)} = \frac{1}{2}D^H_{1111}$
Vertical strain $\overline{\varepsilon}^{(2)} = [0 \quad 1 \quad 0]^T$	$Q^{(2)} = \frac{1}{2}D^H_{2222}$
Shear strain $\overline{\varepsilon}^{(3)} = [0 \quad 0 \quad 1]^T$	$Q^{(3)} = \frac{1}{2}D^H_{1212}$
Horizontal and vertical strain $\overline{\varepsilon}^{(4)} = [1 \quad 1 \quad 0]^T$	$Q^{(4)} = \frac{1}{2}\left(2D^H_{1122} + D^H_{1111} + D^H_{2222}\right)$

According to Table 1, the effective elastic tensor D^H can be expressed as

$$D^H = \begin{bmatrix} D^H_{1111} & D^H_{1122} & 0 \\ D^H_{1122} & D^H_{2222} & 0 \\ 0 & 0 & D^H_{1212} \end{bmatrix} = \begin{bmatrix} 2Q^{(1)} & Q^{(4)} - Q^{(2)} - Q^{(1)} & 0 \\ & 2Q^{(2)} & 0 \\ sym & & 2Q^{(3)} \end{bmatrix} \tag{9}$$

2.2 Sensitivity analysis of the effective elastic properties

It is critical to acquire gradient information of the design variables to guide the optimal algorithm to search for an optimum solution efficiently during the iteration process, which is an important step in topology optimization. In this regard, topological sensitivity is frequently defined as the derivative with respect to design variable, which in the density-based finite element framework is the relative density of element. In order to derive the sensitivities with respect to the elastic properties of the macro-materials, its Young's modulus can be interpolated as the function of the element density as

$$E_e = E(x_e) = x_e^p E_0, \ 0 < x_{\min} \le x_e \le 1 \tag{10}$$

Where E_e is the elastic modulus of element *e* with density interpolation. x_e designates the relative density of the element *e*, which takes values between 0 and 1. p is a penalization factor (typically p = 3-5) introduced to ensure the density distribution closer towards the black-and-white solutions. E_0 denotes the elastic modulus of solid material. $x_{\min}$ is a small value of the density of element, e.g. 0.001, to avoid the singularity of the stiffness matrix.

As shown in Table 1, the strain energy of microstructure under corresponding boundary condition n is therefore stated as

$$Q^{(n)} = \frac{1}{2} U^{(n)T} K U^{(n)} \tag{11}$$

Based on Eq.(11), the gradient of strain energy microstructure respect to design variable x_i can be expressed as follows

$$\begin{aligned} \frac{\partial Q^{(n)}}{\partial x_i} &= \frac{\partial}{\partial x_i}\left(\frac{1}{2} F^{(n)T} U^{(n)}\right) = \frac{\partial}{\partial x_i}\left(\frac{1}{2} U^{(n)T} K U^{(n)}\right) \\ &= \frac{1}{2}\left[U^{(n)T} \frac{\partial K}{\partial x_i} U^{(n)} + 2\frac{\partial U^{(n)T}}{\partial x_i} K U^{(n)}\right] \\ &= \frac{1}{2} U^{(n)T} \frac{\partial K}{\partial x_i} U^{(n)} = \frac{P}{x_i}\left(\frac{1}{2} U_i^{(n)T} K_i U_i^{(n)}\right) = \frac{P}{x_i} Q_i^{(n)} \end{aligned} \tag{12}$$

Where

$$\begin{aligned} \frac{\partial U^{(n)T}}{\partial x_i} K U^{(n)} &= \begin{bmatrix} \frac{\partial U_\Gamma^{(n)T}}{\partial x_i} & \frac{\partial U_\Omega^{(n)T}}{\partial x_i} \end{bmatrix} \begin{bmatrix} F_\Gamma^{(n)} \\ F_\Omega^{(n)} \end{bmatrix} \\ &= \begin{bmatrix} 0 & \frac{\partial U_\Omega^{(n)T}}{\partial x_i} \end{bmatrix} \begin{bmatrix} F_\Gamma^{(n)} \\ 0 \end{bmatrix} = 0 \end{aligned} \tag{13}$$

$U_\Gamma^{(n)}$ is the nodal displacement vector on the boundary of the microstructure, $U_\Omega^{(n)}$ is the inner nodal displacement vector. $F_\Gamma^{(n)}$ is the nodal force vector on the boundary, $F_\Omega^{(n)}$ is the inner nodal force vector inside the microstructure.

According to Eqs. (9) and (12), the sensitivity of effective elastic tensor can be obtained.

$$\frac{\partial D^H}{\partial x_i} = \begin{bmatrix} \frac{\partial D_{1111}^H}{\partial x_i} & \frac{\partial D_{1122}^H}{\partial x_i} & 0 \\ & \frac{\partial D_{2222}^H}{\partial x_i} & 0 \\ sym & & \frac{\partial D_{1212}^H}{\partial x_i} \end{bmatrix} = \frac{P}{x_i}\begin{bmatrix} 2Q_i^{(1)} & Q_i^{(4)} - Q_i^{(2)} - Q_i^{(1)} & 0 \\ & 2Q_i^{(2)} & 0 \\ sym & & 2Q_i^{(3)} \end{bmatrix} \tag{14}$$

3. Topology optimization model of the material microstructures

3.1 Topology optimization model with extreme elastic properties

With regard to topology optimization of the material microstructure with the extreme properties, the design of the microstructural unit cell with the maximum shear modulus or bulk modulus are the most representative examples. Based on the SIMP interpolation model and the design variable of elemental relative density, the optimization problem can be formulated as properly distributing the solid material in the unit cell of the microstructure subject to a given material volume so that the effective shear or bulk modulus approaches its possible maximum value. Thus, the optimization problem can be mathematically stated as follows

$$\begin{cases} find \ \ \mathbf{x}_e \ \ (e=1,2,\ldots,N) \\ Max \ \ \ G \ or \ K \\ s.t. \quad V(x)/V_0 - f = 0 \\ \qquad 0 \le x_e \le 1 \end{cases} \tag{15}$$

Where x_e is elemental relative density, i.e. design variable, and G、K is the shear and bulk modulus of microstructural unit cell respectively, i.e. optimization objective. $V(x)$ is the volume of the optimized structure and V_0 is the given total structural volume. f is the allowable material volume fraction of the unit cell.

According to Eq.(9), the shear modulus G and the bulk modulus K of the microstructural unit cell can be expressed as

$$G = D^H_{1212} \tag{16}$$

$$K = \frac{1}{4}\left(D^H_{1111} + D^H_{1122} + D^H_{2211} + D^H_{2222}\right) \tag{17}$$

According to Eq.(14), the sensitivity of bulk modulus $\frac{\partial K}{\partial x_e}$ and shear modulus $\frac{\partial G}{\partial x_e}$ of the microstructural unit cell with respect to the design variable x_e can be expressed as

$$\frac{\partial G}{\partial x_e} = \frac{\partial D^H_{1212}}{\partial x_e} = \frac{2P}{x_e} Q_e^{(3)} \tag{18}$$

$$\frac{\partial K}{\partial x_e} = \frac{1}{4}\left(\frac{\partial D^H_{1111}}{\partial x_e} + \frac{\partial D^H_{1122}}{\partial x_e} + \frac{\partial D^H_{2211}}{\partial x_e} + \frac{\partial D^H_{2222}}{\partial x_e}\right) = \frac{P}{2x_e} Q_e^{(4)} \tag{19}$$

3.2 Topology optimization model with prescribed elastic properties

With regard to topology optimization of the microstructural unit cell with the prescribed properties, the design of the microstructural unit cell with the prescribed Poisson's ratio are the most representative examples.

For simplicity but without losing any generality, this paper focus on the design of microstructural unit cell subject to the plane stress condition, thus the effective elastic tensor of the microstructural unit cell can be written as

$$D^H=\begin{bmatrix} D_{11}^H & D_{12}^H & 0 \\ D_{12}^H & D_{22}^H & 0 \\ 0 & 0 & D_{33}^H \end{bmatrix}=\begin{bmatrix} \frac{E}{1-\mu^2} & \frac{E\mu}{1-\mu^2} & 0 \\ \frac{E\mu}{1-\mu^2} & \frac{E}{1-\mu^2} & 0 \\ 0 & 0 & \frac{E}{2(1+\mu)} \end{bmatrix}=\frac{E}{1-\mu^2}\begin{bmatrix} 1 & \mu & 0 \\ \mu & 1 & 0 \\ 0 & 0 & \frac{1-\mu}{2} \end{bmatrix} \quad (20)$$

For convenience, the factor of the matrix is set as an constant $\beta = E/1-\mu^2$. So, the effective Poisson's ratio of the microstructural unit cell can be obtain from the Eq.(20), and be expressed as follow

$$\mu=\frac{D_{12}^H}{D_{11}^H}=\frac{D_{12}^H}{D_{22}^H} \quad (21)$$

The Poisson's ratio μ of the material is within the interval $-1 \le \mu \le 1$ for plane stress problems in the classic theory of elasticity[2]. In order to fully demonstrate the effectiveness of the proposed method, the Poisson's ratio μ is set to -1, -0.5, -0.3, 0, 0.3, 0.5 and 1 respectively as the optimization objective.

According to Eq.(21), the optimal microstructure configuration with the prescribed Poisson's ratio μ can be obtain through solving the optimization model of the microstructure with prescribed properties(i.e. D_{11}^H and D_{12}^H are prescribed).The properties of $D_{11}^H = D_{22}^H = 1$ and $\mathrm{D}_{12}^H = \mathrm{D}_{21}^H = \mu$ are prescribed in this paper, so as to obtain the optimal microstructure with the prescribed effective elastic tensor as follows

$$\mathrm{D}^{H*}=\begin{bmatrix} D_{11}^{H*} & D_{12}^{H*} & 0 \\ D_{21}^{H*} & D_{22}^{H*} & 0 \\ 0 & 0 & D_{66}^H \end{bmatrix}=\begin{bmatrix} 1 & \mu & 0 \\ \mu & 1 & 0 \\ 0 & 0 & D_{66}^H \end{bmatrix} \quad (22)$$

In order to generate optimal microstructural configuration with the prescribed properties, the objective function is defined as the minimization of the sum of squared difference between D^H and the prescribed elastic tensor $\mathrm{D}^{\mathrm{H}*}$. Thus, the optimization problem can be formulated as follows

$$\begin{cases} find \ \ \mathbf{x}_e \ \ (e=1,2,...,N) \\ Min \ \ \varphi=\frac{1}{2}\sum_{k,l=1}^{3}\eta_{kl}(\mathbf{D}_{kl}^H(x_e)-\mathbf{D}_{kl}^{H*})^2 \\ s.t. \ \ \ V(x)/V_0 - f = 0 \\ \qquad 0 \le \mathbf{x}_e \le 1 \end{cases} \quad (23)$$

Where η_{kl} is the weighting factor associated with corresponding component of the effective elastic tensor, $\eta_l = [0.01 \quad 0.01 \quad 1]$ in this paper. $V(x)$ is the volume of the optimized structure and V_0 is the given total structural volume. f is the allowable material volume fraction of the unit cell.

According to Eq.(14), the sensitivity of the objective function $\frac{\partial \varphi}{\partial \mathrm{x_e}}$ with respect to the design variable x_e can be expressed as

$$\begin{aligned}
&\frac{\partial \varphi}{\partial x_e}=\sum_{l=1}^{3}\eta_l(\mathbf{D}_{ll}^H(x_e)-\mathbf{D}_{ll}^{H*})\frac{\partial \mathbf{D}_{ll}^H}{\partial x_e} \\
&=\eta_1\left(\mathbf{D}_{11}^H(x_e)-\mathbf{D}_{11}^{H*}\right)\frac{2P}{x_e}Q_e^{(1)}+ \\
&\eta_2\left(\mathbf{D}_{22}^H(x_e)-\mathbf{D}_{22}^{H*}\right)\frac{2P}{x_e}Q_e^{(2)}+ \\
&\eta_3\left(\mathbf{D}_{12}^H(x_e)-\mathbf{D}_{12}^{H*}\right)\frac{P}{x_e}\left(Q_e^{(4)}-Q_e^{(2)}-Q_e^{(1)}\right)
\end{aligned} \tag{24}$$

4. **Numerical implementation**

In this paper, the periodic microstructural unit cell with extreme property or prescribed property can be obtained based on topology optimization technique and energy-based homogenization method. With the help of the finite element analysis technique, corresponding sensitivity analysis procedure mentioned above and optimality criteria (OC) method, the optimization model can be solved to evolve the microstructure of cellular material to an optimum. The convergence criterion is defined in terms of the change in the consecutive cycles over two iteration step as $\left|x^{(k+1)}-x^k\right|\le\delta$, where δ is a allowable convergence threshold which is set to be 0.01 throughout this paper. The whole optimization procedure for the design of microstructure unit cell of cellular material can be described by the flowchart in Fig. 2 and outlined as follows

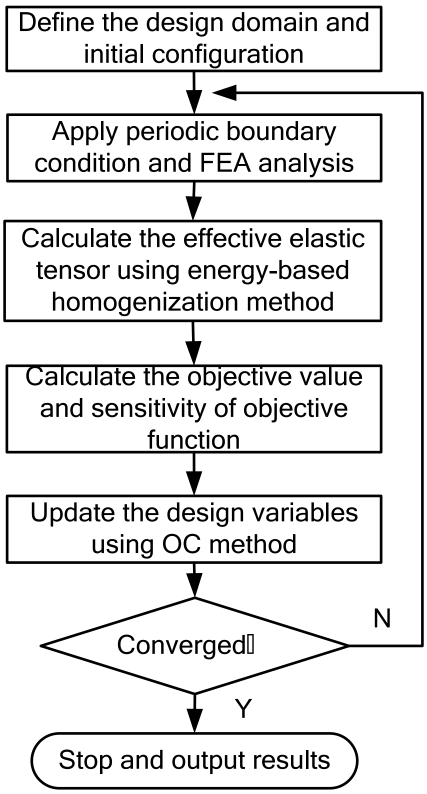


Fig. 2 Flowchart of the optimization procedure

Step 1: Define the design domain and optimization parameters with the volume fraction, filter radius and penalty factor. Discretize the periodic design domain using finite element mesh and construct initial configuration.

Step 2: Apply periodic boundary conditions. Carry out finite element analysis and output the corresponding strain displacement field.

Step 3: Calculate the effective elastic tensor based on the energy-based homogenization method.

Step 4: Calculate the objective value and the sensitivity of the objective function on the design variables

Step 5: Update the design variables using optimality criteria method.

Step 6: Judge the absolute value of the change in the consecutive cycles of the optimization. If the absolute value of the difference is less than the allowable convergence threshold, then converge, output the result, otherwise, repeat the step 2 to step 5.

The design of material microstructures highly depend on the optimization parameters and optimization algorithm, which lead to the numerical problem that the objective function is hard to converge and the optimization parameters is hard to select[1]. This is mainly because of the fact that there are multiple solutions in the design of microstructures, i.e. different microstructures could possess the same physical property[1]. Moreover, the applied periodic boundary conditions would result in a uniformly distributed sensitivity field, thus making the design variable update more impossible. So the initial distribution would be design specifically based on engineer's experience at the beginning of the optimization iteration, which could increase the inhomogeneity of the design domain and have certain guidance on the optimal microstructure configuration, so as to guide the direction of optimization iterative possess , prevent the multiple solutions from emerging during the material design procedure, and accelerate the update of design variables, which benefit the reduction of the sensitivity of optimization algorithm on the optimization parameters and the improvement of computational efficiency. According to the geometric symmetry and the number of holes in the design domain, several typical initial configurations are shown in the Fig. 3.

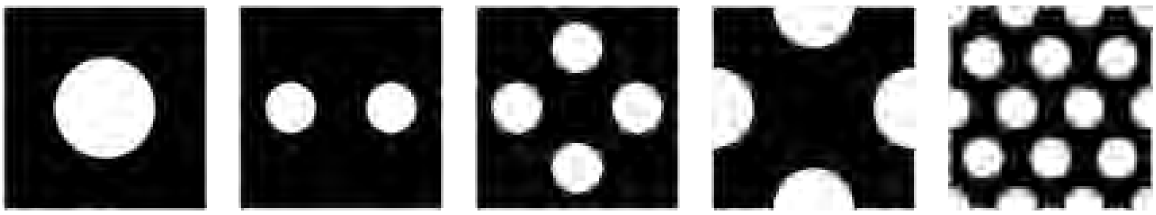


Fig.3. Different initial design configuration

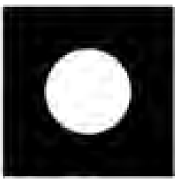
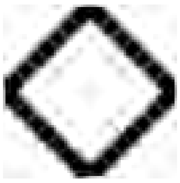
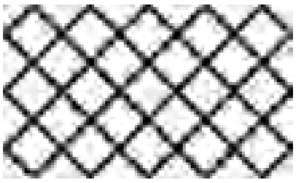
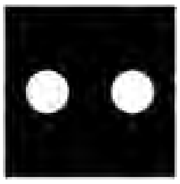
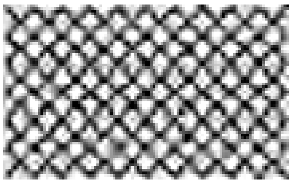
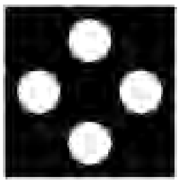
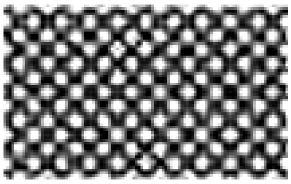
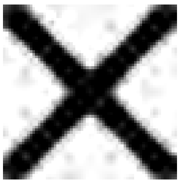
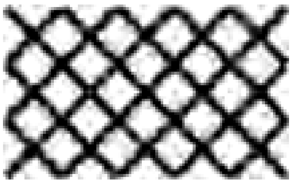
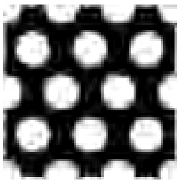
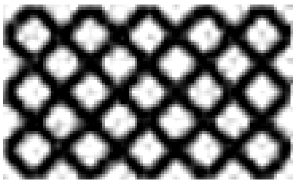
5. Numerical examples and discussion

In all the examples of this section, the Young's moduli and Poisson's ratio of the solid material are selected as $E = 9.1$ and $\mu = 0.3$ respectively. The design domain of the unit cell of microstructure is discretized into 40×40 four-node square elements (Q4). The black region in the distribution represents the solid material part and the white region represents the holes (namely the void regions), the gray region represents the intermediate density area.

5.1 Cellular material microstructures with extreme elastic property

When considering the various volume fraction and initial design configuration, the optimal microstructure with extreme shear modulus and corresponding effective elasticity matrixes are shown in Table 2.

Table 2 Optimal microstructures and effective elasticity matrixes of cellular materials with extreme shear modulus for various volume fraction and initial configuration.

Initial configuration	Volume fraction	Optimal topology configuration 1×1	3×5	Effective elasticity matrixes D^H
	0.25			$\begin{bmatrix} 0.5798 & 0.5592 & 0 \\ 0.5592 & 0.5798 & 0 \\ 0 & 0 & 0.5128 \end{bmatrix}$ $G = 0.5128$
	0.4			$\begin{bmatrix} 1.0701 & 0.9228 & 0 \\ 0.9228 & 1.0422 & 0 \\ 0 & 0 & 0.8358 \end{bmatrix}$ $G = 0.8358$
	0.55			$\begin{bmatrix} 1.9410 & 1.4364 & 0 \\ 1.4364 & 1.9410 & 0 \\ 0 & 0 & 1.2762 \end{bmatrix}$ $G = 1.2762$
	0.4			$\begin{bmatrix} 1.0720 & 0.9613 & 0 \\ 0.9613 & 1.0720 & 0 \\ 0 & 0 & 0.8611 \end{bmatrix}$ $G = 0.8611$
	0.55			$\begin{bmatrix} 2.0284 & 1.5043 & 0 \\ 1.5043 & 2.0283 & 0 \\ 0 & 0 & 1.3351 \end{bmatrix}$ $G = 1.3351$

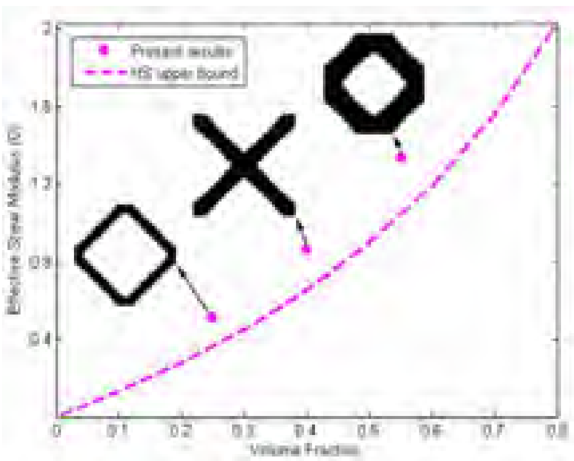


Fig. 4. Comparison between the current solutions and HS upper bound

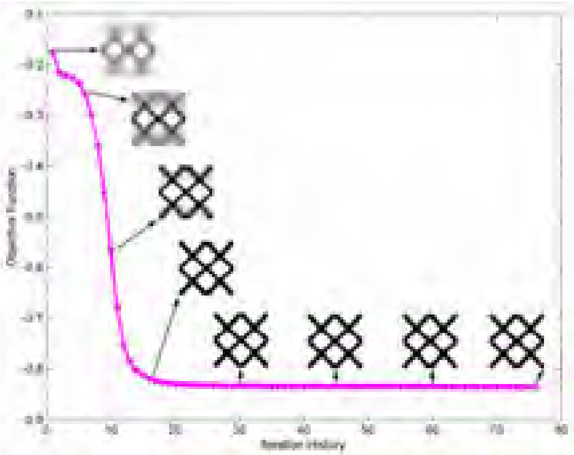


Fig. 5 The iterative curve of microstructures for maximizing shear modulus, volume=0.4, Initial=2

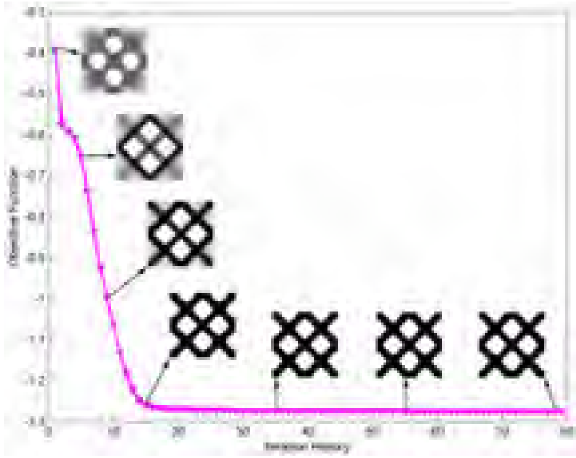


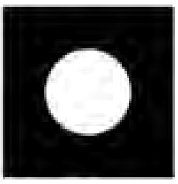
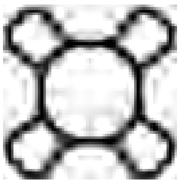
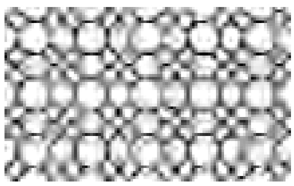
Fig. 6 The iterative curve of microstructures for maximizing shear modulus, volume=0.55, Initial=3

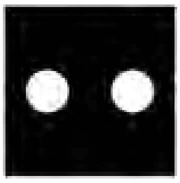
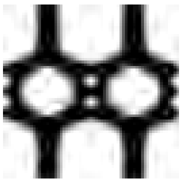
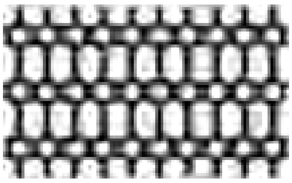
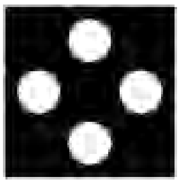
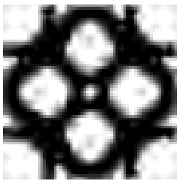
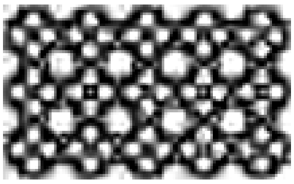
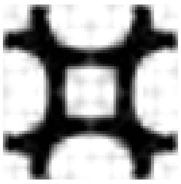
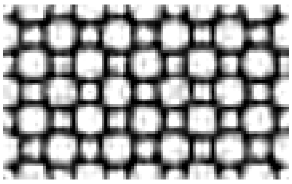
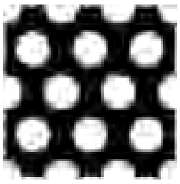
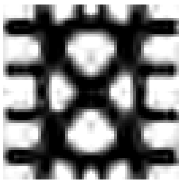
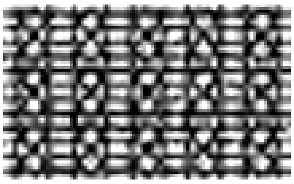
When the volume fractions are set to be 0.25, 0.40, 0.55 of the design domain respectively, the corresponding shear modulus values for different initial design configuration are 0.5128, 0.8611, 1.3351. As can be seen from Fig. 6, all the value of effective shear modulus exceed the corresponding Hashin-Shtrikman upper bound when the optimization objective of this example is to obtain the microstructures of cellular material with extreme shear modulus, which is in good agreement with the conclusion of reference [33] that the Hashin-Shtrikman upper and lower bound formulation is not the best choice for predicting the macroscopic effective shear modulus of composite materials. It also verifies the correctness and reliability of the proposed method for the design of extreme shear modulus of the microstructure.

When the volume fraction is set to be same, the values of extreme shear modulus for various initial design configurations are almost the same and the iterative process is stably convergent. For example, when the the volume fraction is set to 0.4, the extreme shear modulus of material microstructure is 0.8358 and 0.8611 respectively for the initial design configuration of Initial=2 and Initial=4. Similarly, when the the volume fraction is set to 0.55, the extreme shear modulus of material microstructure is 1.2762 and 1.3351 respectively for the initial design configuration of Initial=3 and Initial=5.

Fig. 5 and Fig. 6 shows the iteration histories of the objective function under the volume fraction 0.40, Initial=2 and the volume fraction 0.55, Initial=3 respectively. It can be found that the objective function stably and rapidly converge to their final solutions. And it can be concluded that the initial design configuration is necessary and effective to prevent the multiple solutions from emerging, restrain a uniform distribution of sensitivity field from being obtained, and avoid the oscillation of the iterative process, which will benefit the computational efficiency. A number of numerical experiments indicate that the sensitivity of optimization parameters for the optimization algorithm is reduced under the various initial design configurations.

Table 3 Optimal microstructures and effective elasticity matrixes of cellular materials with extreme bulk modulus for various volume fraction and initial configuration.

Initial configuration	Volume fraction	Optimal topology configuration		Effective elasticity matrixes D^H
		1×1	3×5	
	0.25			$\begin{bmatrix} 0.3941 & 0.3593 & 0 \\ 0.3593 & 0.3941 & 0 \\ 0 & 0 & 0.0117 \end{bmatrix}$ $K = 0.3767$

	0.4			$\begin{bmatrix} 0.8383 & 0.5839 & 0 \\ 0.5839 & 1.2217 & 0 \\ 0 & 0 & 0.0578 \end{bmatrix}$ $K = 0.8070$
	0.55			$\begin{bmatrix} 1.9464 & 1.0673 & 0 \\ 1.0673 & 1.9464 & 0 \\ 0 & 0 & 0.8156 \end{bmatrix}$ $K = 1.5069$
	0.4			$\begin{bmatrix} 1.0295 & 0.7031 & 0 \\ 0 & 1.0295 & 0 \\ 0 & 0 & 0.0837 \end{bmatrix}$ $K = 0.8663$
	0.55			$\begin{bmatrix} 2.2129 & 0.7910 & 0 \\ 0.7910 & 2.0285 & 0 \\ 0 & 0 & 0.1518 \end{bmatrix}$ $K = 1.4559$

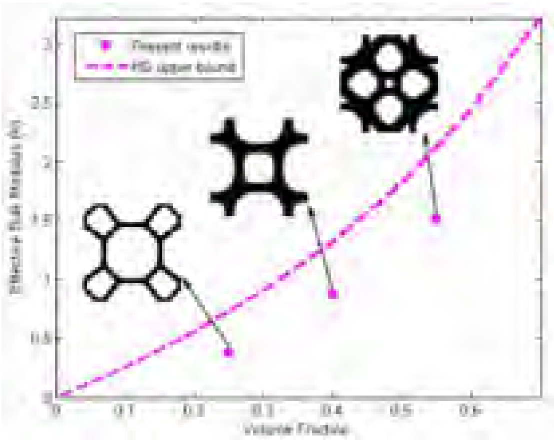


Fig.7. Comparison between the current solutions and HS upper bound

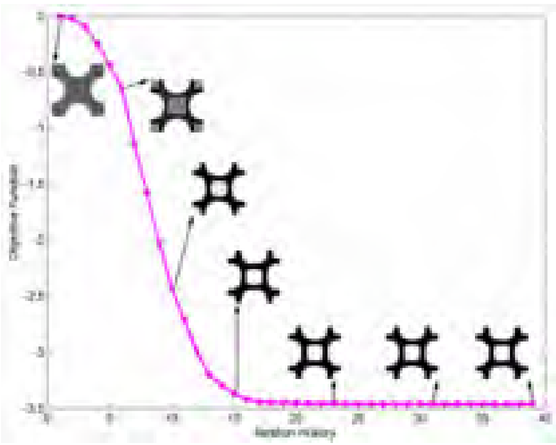


Fig.8. The iterative curve of microstructures for maximizing bulk modulus, volume=0.4,Initial=4

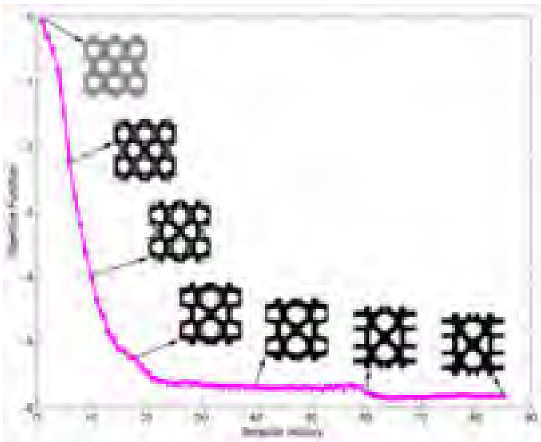


Fig.9. The iterative curve of microstructures for maximizing bulk modulus, volume=0.55,Initial=5

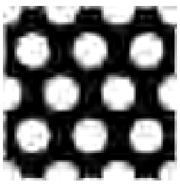
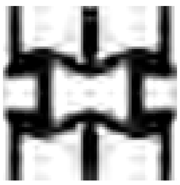
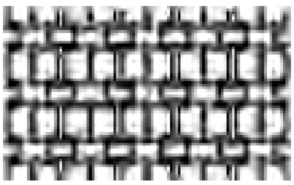
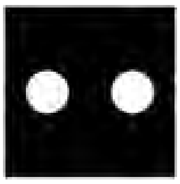
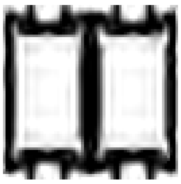
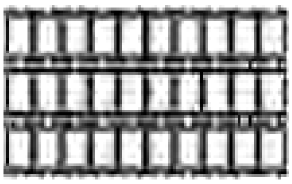
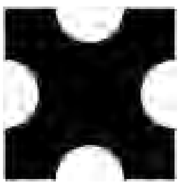
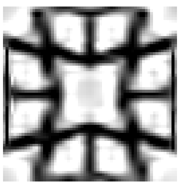
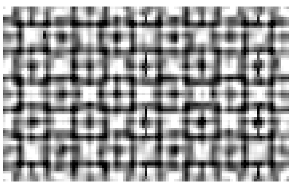
Under the various volume fractions and initial design configurations, the optimal microstructures with extreme bulk modulus and corresponding effective elastic matrixes are shown in Table 3.

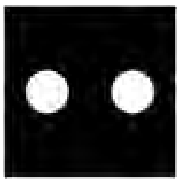
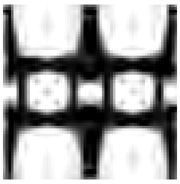
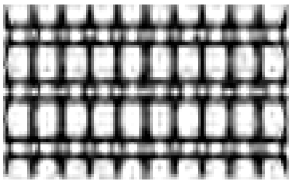
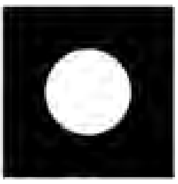
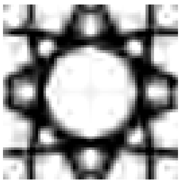
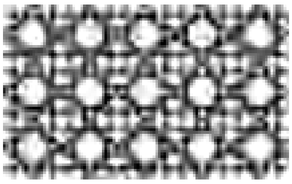
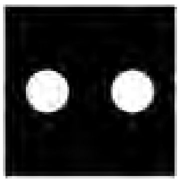
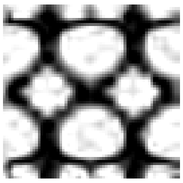
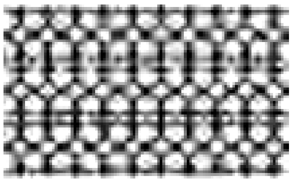
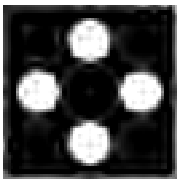
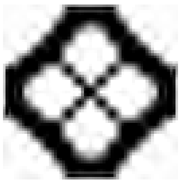
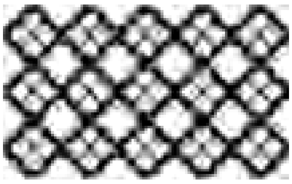
When the volume fractions are set to be 0.25, 0.40, 0.55 of the design domain respectively, the corresponding bulk modulus values for different initial design configurations are 0.3767, 0.8663, 1.5069. As can be seen from Fig. 7, all the value of effective bulk modulus are close to the corresponding Hashin-Shtrikman upper bound when the optimization objective of this example is to obtain the microstructures of cellular material with extreme bulk modulus, which is in good agreement with the prediction result for the effective bulk modulus of composite material in the reference [18]. It also verifies the correctness and reliability of the proposed method for the design of extreme bulk modulus of the microstructure.

In accordance with the conclusion that the microstructures with extreme shear modulus is designed, the value of extreme bulk modulus for various initial design configuration are almost the same and the iterative process is stably convergent when the volume fraction is set to be same. The objective function stably and rapidly converges to their final solutions when the initial configuration is designed specifically, as shown in Fig. 8 and Fig. 9. It can be concluded that the initial design configuration is necessary and effective to avoid the oscillation of the iterative process, restrain a uniform distribution of sensitivity field from being obtain, which benefit the improvement of computational efficiency and the reduction of the sensitivity of optimization algorithm on the optimization parameters.

5.2 Cellular material microstructures with prescribed elastic property

Table 4 Optimal microstructures and effective elasticity matrixes of cellular materials with different prescribed Poisson's ratio for different initial configuration

Initial configuration	Prescribed effective Poisson's ratio	Optimal topology configuration		Effective elasticity matrixes D^H
		1×1	3×5	
	-1			$\begin{bmatrix} 0.6685 & -0.4583 & 0 \\ -0.4583 & 0.6689 & 0 \\ 0 & 0 & 0.0193 \end{bmatrix}$ $\mu=-0.6855$
	-0.5			$\begin{bmatrix} 0.7952 & -0.3685 & 0 \\ -0.3685 & 0.7681 & 0 \\ 0 & 0 & 0.0116 \end{bmatrix}$ $\mu=-0.4634$
	-0.3			$\begin{bmatrix} 0.8655 & -0.2727 & 0 \\ -0.2727 & 0.8655 & 0 \\ 0 & 0 & 0.0284 \end{bmatrix}$

				$\mu=-0.3151$
	0			$\begin{bmatrix} 0.5341 & -0.0019 & 0 \\ -0.0019 & 0.4711 & 0 \\ 0 & 0 & 0.0122 \end{bmatrix}$ $\mu=-0.0035$
	0.3			$\begin{bmatrix} 0.6090 & 0.1809 & 0 \\ 0.1809 & 0.6090 & 0 \\ 0 & 0 & 0.0768 \end{bmatrix}$ $\mu=0.2971$
	0.5			$\begin{bmatrix} 0.6173 & 0.3206 & 0 \\ 0.3206 & 0.5717 & 0 \\ 0 & 0 & 0.0385 \end{bmatrix}$ $\mu=0.5193$
	1			$\begin{bmatrix} 0.9871 & 0.9039 & 0 \\ 0.9039 & 0.9871 & 0 \\ 0 & 0 & 0.7026 \end{bmatrix}$ $\mu=0.9157$

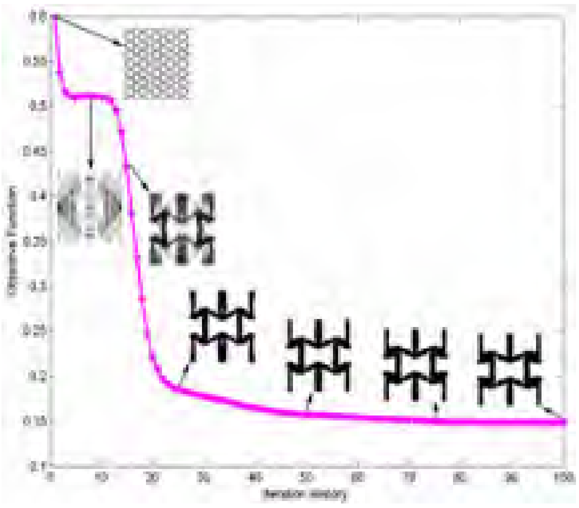


Fig. 10. The iterative curve of microstructures for $\mu=-1$, volume=0.4, Initial=5

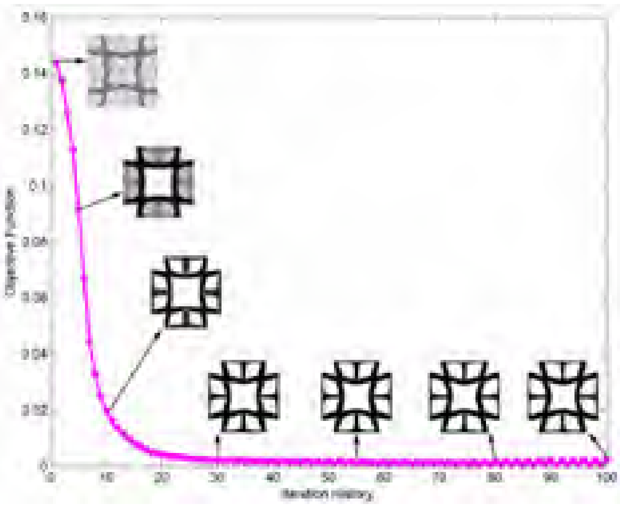


Fig. 11. The iterative curve of microstructures for $\mu=-0.3$, volume=0.4, Initial=4

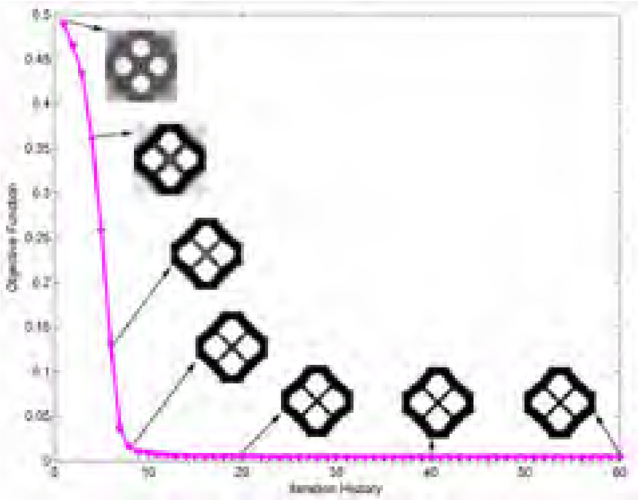


Fig. 12. The iterative curve of microstructures for $\mu = 1$, volume=0.4, Initial=3

The optimal topology configuration and effective elasticity matrix can be obtained using different effective Poisson ratios as the optimization objectives under various initial design configurations, as shown in Table 3. Though the comparative analysis it can be found that the effective Poisson's ratio is $\mu = -0.6855$ when the optimization objective is set to be $\mu = -1$, which is close to the numerical result and similar to the optimal microstructure of the reference[2]. The difference between the optimized result and the prescribed target is relatively smaller when the optimization objective is set to be other prescribed values, and the clear topology configuration also can be obtained.

The iteration histories of the different optimization objectives(such as $\mu = -1$, $\mu = -0.3$, $\mu = 1$)under various initial design configurations (such as Initial=5、Initial=4、Initial=3) are shown as Fig.10, Fig.11 and Fig.12 respectively. It can be found that the objective function stably and rapidly converge to their optimal solutions.

The analysis above show that the proposed method is correct and effective to the design of the material microstructures with prescribed properties, and also indicate that the initial design configuration can avoid the oscillation of the objective function effectively and improve the computational efficiency to a great extent.

6. Conclusion

In this paper, an efficient energy-based homogenization method is used to evaluate the effective elastic properties of the periodic microstructure unit cell. The topology optimization technique is utilized to obtain an optimal microstructural configuration with extreme properties or desired properties subject to a volume fraction constraint under five categories of typical initial design configuration. Several 2D examples are presented to demonstrate the effectiveness and correctness of the proposed method in the design of microstructures, and also indicate that the initial design configuration can solve the problem of multiple solutions and avoid the oscillation of the objective function effectively in the iterative process, and this may result in the efficient computational efficiency and the lower sensitivity of the optimization algorithm on the optimization parameters. Many interesting microstructures and the corresponding effective elastic tensors under various initial design configurations are found and presented.

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