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Topology Optimal Design of Material Microstructures Using Strain Energy-based Method

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Abstract

Sensitivity analysis and topology optimization of microstructures using strain energy-based method is presented. Compared with homogenization method, the strain energy-based method has advantages of higher computing efficiency and simplified programming. Both the dual convex programming method and perimeter constraint scheme are used to optimize the 2D and 3D microstructures. Numerical results indicate that the strain energy-based method has the same effectiveness as that of homogenization method for orthotropic materials.

Keywords: strain energy-based method; homogenization method; microstructure design; topology optimization

1 Introduction

It is known that the macro-properties of composite materials depend upon the periodic microstructure, and the materials can be optimized through the layout of material phases within the microstructure to achieve extreme properties such as negative Poisson's ratio, zero or negative thermal expansion coefficients. The application of topology optimization procedure in designing periodic materials with specified properties was firstly developed by Sigmund[1] who used the "inverse homogenization" method. Thereafter, many researchers launched their works in topology optimization of materials. Sigmund et al.[2] designed composite materials with zero or negative thermal expansion coefficients. Gibiansky, Sigmund and Neves et al.[3-4] maximized the properties of materials subject to the constraint of volume fraction of materials. Silva et al.[5-6] performed the optimal design of the piezocomposite microstructure with high performance characteristics. Yin and Yang[7], Yuan and Wu[8] designed periodic materials with prescribed elastic properties. Liu and Cao[9] designed the materials with zero thermal expansions.

Homogenization method is widely used to predict the effective properties of periodic materials and to optimize the microstructures of periodic materials. This method is strictly based on the mathematical theory, but the sensitivity analysis of the effective properties with respect to the element design variables of microstructures is very complicated and time-consuming. This limits the application of homogenization method to some extent. It is therefore necessary to develop more efficient methods for the prediction of the effective elastic properties.

In this paper, the strain energy-based method is developed to predict the effective elastic properties and to calculate the sensitivity of those properties.

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In fact, both the strain energy-based method and homogenization method are equivalent in predicting the effective properties of materials[10] while the sensitivity analysis based on the strain energy-based method is very simple and efficient. The effective elastic properties of orthotropic materials can be evaluated using the strain energy of microstructure under certain loads[11]. In Section 2 of this paper, we define the strain energy-based method and deduce the sensitivity analysis of effective elastic properties correspondingly. The strain energy-based method is then tested and compared with homogenization method. In Section 3, the optimization problem is formulated to design materials with extreme properties. Numerical examples are presented in Section4, followed by some concluding remarks in Section 5.

2 Principle of Strain Energy-Based Method

2.1 Prediction of effective elastic properties of orthotropic materials

The effective properties of periodical composite materials can be characterized by the representative volume element. The periodic microstructure of composite materials can be replaced by an equivalent homogeneous medium with the same volume at the macroscopic level as shown in Fig.1. It satisfies the following conditions: the stress and the strain tensors of the homogeneous medium are equivalent to the average stress and strain of the microstructure with $\frac{1}{V}\int \boldsymbol{\sigma}\mathrm{d}V = \overline{\boldsymbol{\sigma}}$ and $\frac{1}{V}\int \boldsymbol{\varepsilon}\mathrm{d}V = \overline{\boldsymbol{\varepsilon}}$, where V denotes the volume of the representative volume element. The average stress and strain of the homogeneous medium follow the Hooke's law

$$\overline{\boldsymbol{\sigma}} = \boldsymbol{D}^{\mathrm{H}}\overline{\boldsymbol{\varepsilon}} \tag{1}$$

where $\boldsymbol{D}^{\mathrm{H}}$ is the effective elastic tensor of the material.

The effective elastic tensor of 2D orthotropic material can be written in matrix form as

$$\boldsymbol{D}^{\mathrm{H}} = \begin{bmatrix} D_{1111}^{\mathrm{H}} & D_{1122}^{\mathrm{H}} & 0 \\ D_{1122}^{\mathrm{H}} & D_{2222}^{\mathrm{H}} & 0 \\ 0 & 0 & D_{1212}^{\mathrm{H}} \end{bmatrix} \tag{2}$$

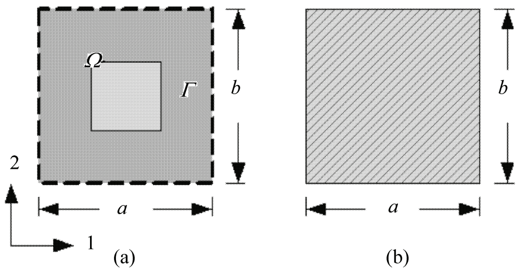


Fig.1 Homogenization of 2D microstructure. (a) microstructure; (b) homogenized microstructure.

Besides, the strain energies stored in microstructure and the hom ogeneous medium have to be equal

$$E(\boldsymbol{\varepsilon}) = \frac{1}{2V}\int_{\Omega}(\sigma_{11}\varepsilon_{11} + \sigma_{22}\varepsilon_{22} + \sigma_{12}\varepsilon_{12})\mathrm{d}\Omega = \frac{1}{2}(\overline{\sigma}_{11}\overline{\varepsilon}_{11} + \overline{\sigma}_{22}\overline{\varepsilon}_{22} + \overline{\sigma}_{12}\overline{\varepsilon}_{12}) = E(\overline{\boldsymbol{\varepsilon}}) \tag{3}$$

Here, $E(\boldsymbol{\varepsilon})$ and $E(\overline{\boldsymbol{\varepsilon}})$ denote the strain energies stored in the microstructure and the homogeneous medium respectively.

Based on Eqs.(2) and (3), the effective elastic tensor can be identified from the strain energies of microstructure under the specific boundary conditions. For example, in the 1st load case, suppose the average strain of the microstructure is $\overline{\boldsymbol{\varepsilon}}^{(1)} = (1\ 0\ 0)^{\mathrm{T}}$, the average stress tensors is $\overline{\boldsymbol{\sigma}}^{(1)} = (D_{1111}^{\mathrm{H}}\ D_{1122}^{\mathrm{H}}\ 0)^{\mathrm{T}}$ correspondingly. Then, the component D_{1111}^{H} can be obtained as: $D_{1111}^{\mathrm{H}} = 2E^{(1)}$. In order to calculate the effective elastic properties, four different boundary conditions are considered as detailed in Table 1.

From Table 1, the $\boldsymbol{D}^{\mathrm{H}}$ can be obtained as

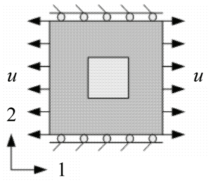
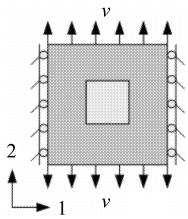
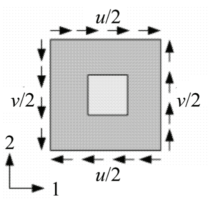
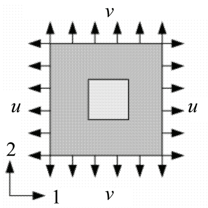
$$\boldsymbol{D}^{\mathrm{H}} = \begin{bmatrix} 2E^{(1)} & E^{(4)} - E^{(2)} - E^{(1)} & 0 \\ & 2E^{(2)} & 0 \\ \text{sym} & & 2E^{(3)} \end{bmatrix} \tag{4}$$

Similarly, effective elastic properties of 3D orthotropic materials can be calculated by the strain energies of microstructures under specific boundary conditions.

2.2 Sensitivity analysis of the effective elastic properties

Suppose the microstructure is discretized by n

Table 1 Boundary conditions and corresponding strain energies of microstructures

Boundary condition	Average strain tensor	Strain energy
	$\bar{\boldsymbol{\varepsilon}}^{(1)}=\begin{pmatrix}1\\0\\0\end{pmatrix}$	$E^{(1)}=\frac{1}{2}D_{1111}^{\mathrm{H}}$
	$\bar{\boldsymbol{\varepsilon}}^{(2)}=\begin{pmatrix}0\\1\\0\end{pmatrix}$	$E^{(2)}=\frac{1}{2}D_{2222}^{\mathrm{H}}$
	$\bar{\boldsymbol{\varepsilon}}^{(3)}=\begin{pmatrix}0\\0\\1\end{pmatrix}$	$E^{(3)}=\frac{1}{2}D_{1212}^{\mathrm{H}}$
	$\bar{\boldsymbol{\varepsilon}}^{(4)}=\begin{pmatrix}1\\1\\0\end{pmatrix}$	$E^{(4)}=\frac{1}{2}(2D_{1122}^{\mathrm{H}}+D_{1111}^{\mathrm{H}}+D_{2222}^{\mathrm{H}})$

finite elements and the stiffness of element t, $\boldsymbol{K}_t$, can be written in the form of SIMP model

$$\boldsymbol{K}_t = x_t^p \boldsymbol{K}_0 \tag{5}$$

where $x_t \in [0\ \ 1]$ is the density variable of element t. $x_t = 1$ means that the element is full of solid materials and $x_t = 0$ means a void element. $\boldsymbol{K}_0$ is the solid element stiffness. The exponent p is the penalty factor that is often chosen to be $p = 4$.

The equilibrium equation of the finite element is

$$\boldsymbol{KU} = \boldsymbol{F} \tag{6}$$

where $\boldsymbol{U}$ and $\boldsymbol{F}$ are the load vector and displacement vector of element nodes, respectively.

The strain energy of microstructure under boundary condition n is therefore as follows

$$E^{(n)} = \frac{1}{2}\boldsymbol{U}^{(n)\mathrm{T}}\boldsymbol{KU}^{(n)} \tag{7}$$

From Eqs.(6) and (7), the sensitivity of the strain energy with respect to design variable x_t can be obtained

$$\frac{\partial E^{(n)}}{\partial x_t} = \frac{\partial}{\partial x_t}\left(\frac{1}{2}\boldsymbol{F}^{(n)\mathrm{T}}\boldsymbol{U}^{(n)}\right) = \frac{\partial}{\partial x_t}\left(\frac{1}{2}\boldsymbol{U}^{(n)\mathrm{T}}\boldsymbol{KU}^{(n)}\right) = \frac{1}{2}\left[\boldsymbol{U}^{(n)\mathrm{T}}\frac{\partial \boldsymbol{K}}{\partial x_t}\boldsymbol{U}^{(n)} + 2\frac{\partial \boldsymbol{U}^{(n)\mathrm{T}}}{\partial x_t}\boldsymbol{KU}^{(n)}\right] = \frac{1}{2}\boldsymbol{U}^{(n)\mathrm{T}}\frac{\partial \boldsymbol{K}}{\partial x_t}\boldsymbol{U}^{(n)} \tag{8}$$

where

$$\frac{\partial \boldsymbol{U}^{(n)\mathrm{T}}}{\partial x_t}\boldsymbol{KU}^{(n)} = \begin{bmatrix}\frac{\partial \boldsymbol{U}_{\Gamma}^{(n)\mathrm{T}}}{\partial x_t} & \frac{\partial \boldsymbol{U}_{\Omega}^{(n)\mathrm{T}}}{\partial x_t}\end{bmatrix}\begin{bmatrix}\boldsymbol{F}_{\Gamma}^{(n)}\\ \boldsymbol{F}_{\Omega}^{(n)}\end{bmatrix} = \begin{bmatrix}0 & \frac{\partial \boldsymbol{U}_{\Omega}^{(n)\mathrm{T}}}{\partial x_t}\end{bmatrix}\begin{bmatrix}\boldsymbol{F}_{\Gamma}^{(n)}\\ 0\end{bmatrix} = 0 \tag{9}$$

Here $\boldsymbol{U}_{\Gamma}^{(n)}$ and $\boldsymbol{F}_{\Gamma}^{(n)}$ are the nodal displacement vector and force vector on the boundary. $\boldsymbol{U}_{\Omega}^{(n)}$ and $\boldsymbol{F}_{\Omega}^{(n)}$ are the nodal displacement vector and force vector inside.

With the combination of Eqs.(5), (8) and (9), the sensitivity of strain energy can be calculated by

$$\frac{\partial E^{(n)}}{\partial x_t} = \frac{1}{2}\boldsymbol{U}^{(n)\mathrm{T}}\frac{\partial \boldsymbol{K}}{\partial x_t}\boldsymbol{U}^{(n)} = \frac{p}{x_t}\left(\frac{1}{2}\boldsymbol{U}_t^{(n)\mathrm{T}}\boldsymbol{K}_t\boldsymbol{U}_t^{(n)}\right) = \frac{p}{x_t}E_t^{(n)} \tag{10}$$

The sensitivity of effective elastic matrix $\boldsymbol{D}^{\mathrm{H}}$ can be expressed as

$$\frac{\partial \boldsymbol{D}^{\mathrm{H}}}{\partial x_t} = \begin{pmatrix}\frac{\partial D_{1111}^{\mathrm{H}}}{\partial x_t} & \frac{\partial D_{1122}^{\mathrm{H}}}{\partial x_t} & 0\\ & \frac{\partial D_{2222}^{\mathrm{H}}}{\partial x_t} & 0\\ \mathrm{sym} & & \frac{\partial D_{1212}^{\mathrm{H}}}{\partial x_t}\end{pmatrix} = \frac{p}{x_t}\begin{pmatrix}2E_t^{(1)} & E_t^{(4)}-E_t^{(2)}-E_t^{(1)} & 0\\ & 2E_t^{(2)} & 0\\ \mathrm{sym} & & 2E_t^{(3)}\end{pmatrix} \tag{11}$$

Eq.(11) means the sensitivity of effective elastic tensor only depends on the element strain energy.

2.3 Relationship between the strain energy-based method and homogenization method

Based on the small parameter asymptotic expansion, the effective elastic properties of periodic material can be derived as[12]

$$D_{ijkl}^{\mathrm{H}}=\frac{1}{V}\int_{\Omega}D_{ijpq}\left(\varepsilon_{pq}^{0(kl)}-\varepsilon_{pq}^{(kl)}\right)\mathrm{d}\Omega \tag{12}$$

where $\varepsilon_{pq}^{0(kl)}$ is the homogeneous strain field, and $\varepsilon_{pq}^{(kl)}$ is the periodic solution to the variational type problem

$$\int_{\Omega}D_{ijpq}\varepsilon_{pq}^{(kl)}\frac{\partial\delta\vartheta_i}{\partial y_j}\mathrm{d}\Omega=\int_{\Omega}D_{ijpq}\varepsilon_{pq}^{0(kl)}\frac{\partial\delta\vartheta_i}{\partial y_j}\mathrm{d}\Omega \tag{13}$$

$$(\forall\delta\vartheta_i\in\Omega\ \text{periodicity})$$

The effective elastic properties can be written in its energy form as

$$D_{pqrs}^{\mathrm{H}}\varepsilon_{pq}^{0(kl)}\varepsilon_{rs}^{0(ij)}=\min\frac{1}{V}\int_{\Omega}D_{pqrs}\cdot\left(\varepsilon_{pq}^{0(kl)}-\varepsilon_{pq}^{(kl)}\right)\left(\varepsilon_{rs}^{0(ij)}-\varepsilon_{rs}^{(ij)}\right)\mathrm{d}\Omega \tag{14}$$

As shown in Table 1, the relationship between the effective elastic properties and the strain energy of microstructure in the strain energy-based method can be stated as[13]

$$E(\varepsilon^0)=D_{pqrs}^{\mathrm{H}}\varepsilon_{pq}^{0(kl)}\varepsilon_{rs}^{0(ij)} \tag{15}$$

The combination of Eq.(14) and Eq.(15) results in

$$E\left(\varepsilon^0\right)=\min\frac{1}{V}\int_{\Omega}D_{pqrs}\bullet\left(\varepsilon_{pq}^{0(kl)}-\varepsilon_{pq}^{(kl)}\right)\left(\varepsilon_{rs}^{0(ij)}-\varepsilon_{rs}^{(ij)}\right)\mathrm{d}\Omega \tag{16}$$

It means that the strain energy-based method and homogenization method are just two variants of the same definition of effective material properties[1-2] and they are physically identical.

Based on the homogenization method, the sensitivity analysis of the effective properties with respect to the element density variable x_t can be formulated as

$$\frac{\partial D_{ijkl}^{\mathrm{H}}}{\partial x_t}=\frac{1}{V}\sum_{e=1}^{n}\left(\frac{\partial D_{ijpq}^{e}}{\partial x_t}\varepsilon_{pq}^{0e(kl)}-\frac{\partial(D_{ijpq}^{e}\varepsilon_{pq}^{e(kl)})}{\partial x_t}\right)v_e=\frac{1}{V}\left(\frac{\partial D_{ijpq}^{t}}{\partial x_t}\varepsilon_{pq}^{0t(kl)}v_t-\sum_{e=1}^{n}\frac{\partial(D_{ijpq}^{e}\varepsilon_{pq}^{e(kl)})}{\partial x_t}v_e\right) \tag{17}$$

Compared with Eq.(11), it is relatively complicated for programming. Under the same computing environments (Pentium(R) 4CPU 2.80 GHz, EMS memory 1.00 GB), homogenization method needs 5 min and 38 s for calculating the effective elastic properties and performing sensitivity analysis of microstructure for a model of 400 finite elements, while the proposed method only needs 12 s.

3 Design Microstructures with Extreme Properties

The engineering sign method is used to simplify subscripts involved in the elastic tensor with 11→1, 22→2, 33→3, 23→4, 31→5, 12→6. For example, D_{11}^{H} denotes D_{1111}^{H}.

Microstructures are now designed to maximize effective elastic properties subject to the constraint of material volume fraction and perimeter constraint. The optimization problem can be written as

$$\begin{aligned}&\max\ \ \phi=\sum w_{ij}D_{ij}^{\mathrm{H}}\\&\text{s.t.}\ \ V(\boldsymbol{X})=\sum_{t=1}^{n}x_t v_t\leqslant f\overline{V}\\&\qquad \mathrm{TV}(\boldsymbol{X})=\sum_{r=1}^{m}d_r(x_p-x_q)^2\leqslant\overline{\mathrm{TV}}\\&\qquad 0<\delta\leqslant x_t\leqslant 1\quad t=1,n\end{aligned} \tag{18}$$

where w_{ij} is the weight factor, $V(\boldsymbol{X})$ denotes the total material volume contribution of all elements in the microstructure limited by the upper bound fV_0, f is the volume fraction of material, V_0 is the total volume of the microstructure. A small value of $\delta=10^{-4}$ is used here to avoid the singularity of the elementary matrix during optimization. TV is the so-called total variation that regularizes the solid-void pattern and controls the checkerboard phenomenon simultaneously in the finally obtained microstructure. The role of upper bound $\overline{\mathrm{TV}}$ is twofold: avoidance of checkerboard when $\overline{\mathrm{TV}}$ takes small values and elimination of intermediate values of density variables between 0 and 1 when $\overline{\mathrm{TV}}$ is successively relaxed. The dual convex programming method[14] is used to optimize the 2D and 3D microstructures.

The sensitivity of the objective function with respect to the design variable x_t is

$$\frac{\partial\phi}{\partial x_t}=\sum w_{ij}\frac{\partial D_{ij}^{\mathrm{H}}}{\partial x_t} \tag{19}$$

where $\dfrac{\partial D_{ij}^{\mathrm{H}}}{\partial x_t}$ can be obtained from Eq.(11).

Different objective functions can be defined when w_{ij} takes different values. For example, the optimization problem refers to a single objective optimization of max D_{11}^{H} when $w_{11}=1$, $w_{ij}=0$ ($ij \neq 11$). Alternatively, the optimization problem refers to a bi-objective problem of $\max D_{11}^{\mathrm{H}}+D_{22}^{\mathrm{H}}$ while $w_{11}=w_{22}=0.5$, $w_{ij}=0$ ($ij \neq 11, 22$).

4 Numerical Examples

In this section, 2D and 3D microstructures are designed to maximize the stiffness by the strain energy-based method. Suppose the elastic properties of the isotropic material are $E_{01}=1\ 000$ and $\nu=0.3$, the black and gray regions in the optimal microstructures denote the solid material and void, respectively.

4.1 Single objective optimization for the maximization of microstructure stiffness

For a 2D plane stress problem, the microstructures is discretized with a mesh of 80×80 finite elements. The volume fraction of solid materials is $f=0.5$. The optimal microstructures are shown in Table 2 for different objective functions.

The optimal microstructure related to $\max D_{11}^{\mathrm{H}}$ results in an aligned composite material. The optimal configuration related to the shear stiffness maximization results in a material layout aligned at an angle of 45° in the microstructure. This solution agrees well with the optimal microstructure obtained by the homogenization method[4].

For 3D microstructures, a mesh of 40 × 40 × 40 finite elements is taken into account. When the volume fraction of solid material is $f=0.5$, optimal microstructures with different objective functions are shown in Table 3.

4.2 Multi-objective optimization for the maximization of microstructure stiffness

Considering a combination of horizontal and vertical stiffness defined by $\max w_{11}D_{11}^{\mathrm{H}}+w_{22}D_{22}^{\mathrm{H}}$ for different weight factors, the results of microstructure design are shown in Table 4 for a volume fraction of $f=0.5$.

Table 2 2D optimal microstructures for different optimal objectives

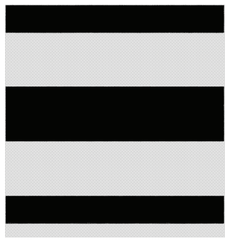
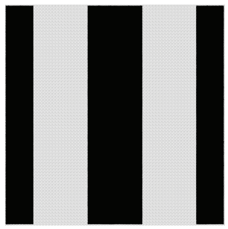
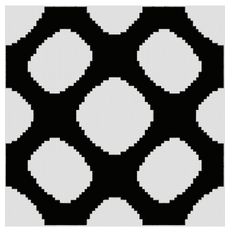
Optimal microstructures	Objectives
	$\max D_{11}^{\mathrm{H}}$ $D_{11}^{\mathrm{H}}=498.0$
	$\max D_{22}^{\mathrm{H}}$ $D_{22}^{\mathrm{H}}=498.0$
	$\max D_{66}^{\mathrm{H}}$ $D_{66}^{\mathrm{H}}=134.7$

Table 3 3D optimal microstructures for different optimal objective functions

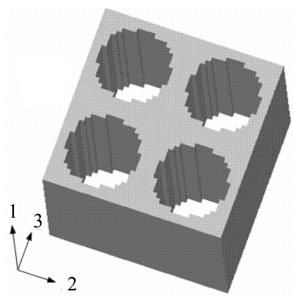
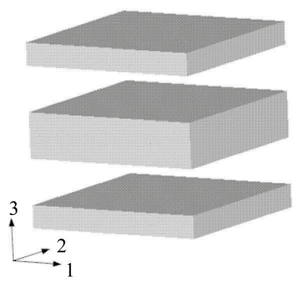
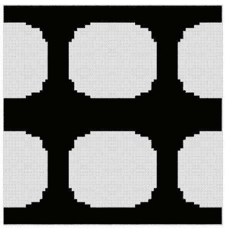
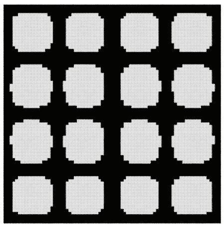
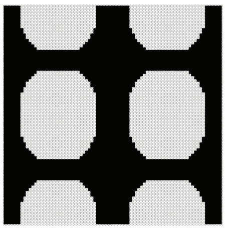
Optimal microstructures	Objectives
	$\max D_{11}^{\mathrm{H}}$ $D_{11}^{\mathrm{H}}=570.6$
	$\max D_{66}^{\mathrm{H}}$ $D_{66}^{\mathrm{H}}=192.3$

Table 4 2D optimal microstructures for multi-objective functions

Optimal microstructures	Objectives
	$\max \frac{3}{5}D_{11}^{H}+\frac{2}{5}D_{22}^{H}$ $D_{11}^{H}=356.6$ $D_{22}^{H}=267.9$
	$\max \frac{1}{2}D_{11}^{H}+\frac{1}{2}D_{22}^{H}$ $D_{11}^{H}=309.9$ $D_{22}^{H}=309.3$
	$\max \frac{2}{5}D_{11}^{H}+\frac{3}{5}D_{22}^{H}$ $D_{11}^{H}=263.0$ $D_{22}^{H}=359.7$

It is shown that different weight factors will produce different optimal microstructures. Besides, 3D microstructures are optimized to maximize the stretch and shear stiffness in three directions for different volume fractions (shown in Table 5).

Obviously, the effective shear stiffness increases and the microstructure becomes more closed as the volume fraction increases. To have a clear idea, the variation of the effective shear term D_{66}^{H} versus the volume fraction f is shown in Fig.2.

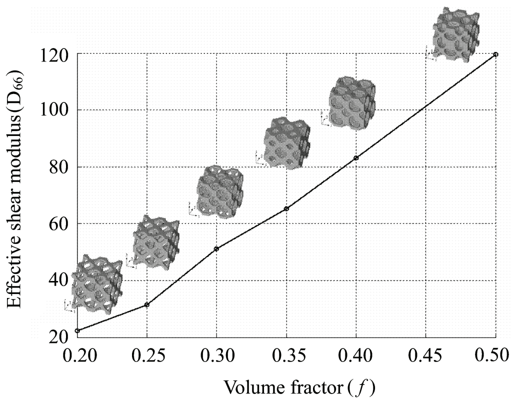
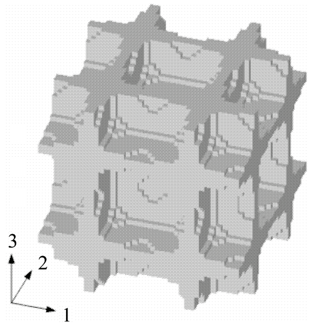
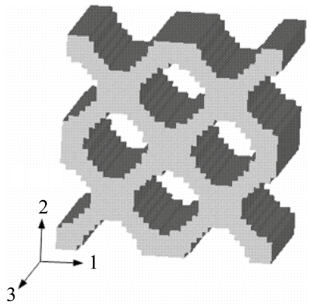
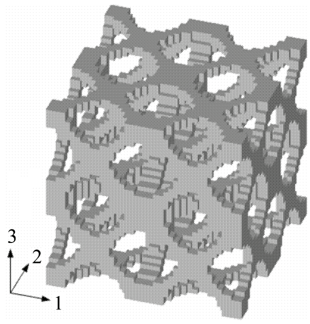
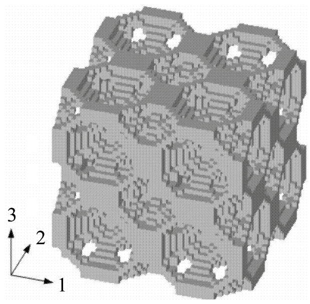
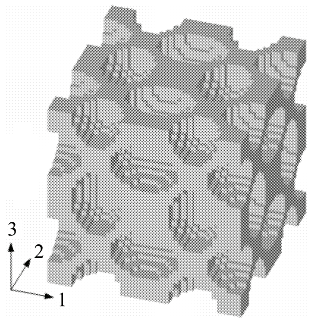


Fig.2 Effective shear modulus versus the volume fraction.

Table 5 3D optimal microstructures for multi-objectives

Optimal microstructures	Objective and volume fractions f
	$\max D_{11}^{H}+D_{22}^{H}+D_{33}^{H}$ $f=0.5$ $D_{11}^{H}=433.5$ $D_{22}^{H}=433.5$ $D_{33}^{H}=433.5$
	$\max D_{33}^{H}+D_{66}^{H}$ $f=0.5$ $D_{33}^{H}=571.3$ $D_{66}^{H}=140.7$
	$\max D_{44}^{H}+D_{55}^{H}+D_{66}^{H}$ $f=0.2$ $D_{44}^{H}=22.35$ $D_{55}^{H}=22.35$ $D_{66}^{H}=22.35$
	$\max D_{44}^{H}+D_{55}^{H}+D_{66}^{H}$ $f=0.3$ $D_{44}^{H}=51.21$ $D_{55}^{H}=51.21$ $D_{66}^{H}=51.21$
	$\max D_{44}^{H}+D_{55}^{H}+D_{66}^{H}$ $f=0.5$ $D_{44}^{H}=119.5$ $D_{55}^{H}=119.5$ $D_{66}^{H}=119.5$

It should be noted that the optimization of microstructures has been studied by many researchers using the "homogenization method". Although the topology optimization of 3D microstructures is theoretically similar to the design of 2D microstructures, design results of 3D microstructures are seldom presented because of the sharp increase of computing time. While the strain energy-based method can avoid this problem and efficiently realize optimal designs of 3D microstructures as presented in Table 5.

5 Conclusions

An efficient method is presented to calculate the effective elastic properties of porous materials in the form of strain energies of microstructures. It is found that the sensitivities with respect to the element variables can be obtained by the scaling of strain energies of the corresponding element. The numerical examples indicate that the optimization results of microstructures using the strain energy-based method are equivalent to that obtained from the homogenization method, but the sensitivity analysis of the proposed method is more simple and efficient. The strain energy-based method is a practical method to realize microstructure optimization and can be widely used in the design of high performance materials in aerospace industries.

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