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Topological design of microstructures of cellular materials for maximum bulk or shear modulus

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ARTICLE INFO

Article history: Received 14 December 2010 Received in revised form 17 January 2011 Accepted 18 January 2011 Available online 12 February 2011

Keywords:
Topology optimization
Homogenization
Cellular material
Bidirectional evolutionary structural
optimization (BESO)
Bulk modulus
Shear modulus

ABSTRACT

This paper presents a new approach to designing periodic microstructures of cellular materials. The method is based on the bidirectional evolutionary structural optimization (BESO) technique. The optimization problem is formulated as finding a micro-structural topology with the maximum bulk or shear modulus under a prescribed volume constraint. Using the homogenization theory and finite element analysis within a periodic base cell (PBC), elemental sensitivity numbers are established for gradually removing and adding elements in PBC. Numerical examples in 2D and 3D demonstrate the effectiveness of the proposed method for achieving convergent microstructures of cellular materials with maximum bulk or shear modulus. Some interesting topological patterns have been found for guiding the cellular material design.

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1. Introduction

Light-weight cellular materials possess various advanced physical, mechanical and thermal properties far beyond solid materials. The properties of cellular materials depend on the way the solid is distributed in the cell. Cellular materials appear widely in nature. Large-scale materials such as honeycombs and metal foams are manufactured through mimicking the natural materials [1]. In the design setting, one wishes to create a new microstructure of a material which produces similar functional properties to those of the natural materials. This objective could be achieved by formulating a topology optimization problem for micro-structural topologies and material properties.

The original topology optimization methods, e.g. homogenization method [2], Solid Isotropic Material with Penalization (SIMP) [3–6], level set method [7–9] and evolutionary structural optimization (ESO) [10,11], were developed to find a stiffest structural layout under given constraints. In the last decade, both SIMP and level set methods have been successfully extended to the design of periodic microstructures of materials or composites [12–17]. Theoretically, the effective physical properties at a specific point in the material can be homogenized (or averaged) by using the homogenization procedure according to its microstructure. The inverse homogenization procedure is to seek a microstructure of a material

with extremal physical properties and the microstructure of the material is represented by a periodic base cell (PBC). Tailoring materials with prescribed constitutive properties, the problem is formulated as an optimization problem where the PBC is modelled with frame elements [12] or solid elements [13,14]. Using the SIMP method, Zhou and Li [15,16] have investigated the computational design of micro-structural composite for extremal conductivity property or graded mechanical property. A level set procedure for the design of electromagnetic meta-materials has been developed by Zhou et al. [17].

ESO was originally developed based on removing inefficient materials from a structure so the resulting topology evolves toward an optimum [10,11]. The later version of the ESO method, namely the bidirectional ESO (BESO), allowed not only removing elements from the least efficient regions, but also adding elements to the most efficient regions simultaneously [18]. However, various weaknesses of the original BESO method [19,20] greatly limit its application to a new engineering field, e.g. the design for material microstructure. Recently, Huang and Xie [21–23] have developed a new and much improved BESO method and successfully overcome these weaknesses. It has been demonstrated that the new BESO method is capable of generating reliable and practical topologies for macro-scale structures with high computational efficiency.

This paper is the first attempt to extend the BESO method to the design of periodic microstructure of cellular material. The advantage of the BESO method is that the structural topology is clearly represented by solid or void elements without grey areas and such

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a topology can be easily manufactured. BESO is also very simple to implement as a "post-processor" to commercial FEA software packages. More importantly, the previous research on material design has indicated that the obtained micro-structural topology depends highly on the used optimization parameters and algorithm [13,14]. This is because of the fact that a number of different microstructures could possess the same physical property. In other words, there is no unique solution for material design. Therefore, it is important to attempt new and different optimization algorithms, such as BESO, in order to find a much wider range of possible solutions to material design.

This paper will focus on the design of a periodic cellular material with maximum bulk or shear modulus under a given volume constraint using BESO. The micro-structural topology and the effective properties of a cellular material are totally represented by PBC which is discretized using finite elements. With the relative ranking of the derived sensitivity number for each iteration, elements within PBC may change from solid (density $x_i = 1$) to void (density $x_i = x_{\min}$) or from void to solid. As a result, the PBC topology will be gradually modified until both volume constraint and the convergent criterion are satisfied. Towards the end of the paper, some 2D and 3D examples will be given to demonstrate the effectiveness of the proposed BESO method.

2. Homogenization and sensitivity analysis

When a cellular material is composed of spatially repeated PBCs and PBC is very small compared with the size of a structural body, the effective elasticity tensor of the macro-material can be found by the homogenization theory [2,24,25] in terms of the material distribution in the domain of PBC, Ω as:

$$E_{ijkl}^{H} = \frac{1}{|Y|} \int_{\Omega} E_{ijpq} (\bar{\varepsilon}_{pq}^{kl} - \tilde{\varepsilon}_{pq}^{kl}) d\Omega$$
 (1)

where |Y| denotes the area (or volume in 3D) of the periodic base cell domain Ω . $\bar{\mathcal{E}}^{kl}_{pq}$ defines the four linearly independent unit strain fields as $\bar{\mathcal{E}}^{11}_{pq} = \begin{pmatrix} 1 & 0 & 0 & 0 \end{pmatrix}^T$, $\bar{\mathcal{E}}^{22}_{pq} = \begin{pmatrix} 0 & 1 & 0 & 0 \end{pmatrix}^T$, $\bar{\mathcal{E}}^{12}_{pq} = \begin{pmatrix} 0 & 0 & 1 & 0 \end{pmatrix}^T$ and $\bar{\mathcal{E}}^{11}_{mn} = \begin{pmatrix} 0 & 0 & 0 & 1 \end{pmatrix}^T$ for 2D cases. The strain fields $\bar{\mathcal{E}}^{kl}_{mn}$ induced by the test strains can be found from the following equation:

$$\int_{\Omega} E_{ijpq} \varepsilon_{ij}(\nu) \tilde{\varepsilon}_{pq}^{kl} d\Omega = \int_{\Omega} E_{ijpq} \varepsilon_{ij}(\nu) \tilde{\varepsilon}_{pq}^{kl} d\Omega$$
 (2)

where $v \in H^1_{per}(\Omega)$ which is the Y-periodic admissible displacement field. Eq. (2) is the weak form of the standard elasticity equation applied to PBC with periodic boundary conditions. This equation is usually solved by finite element analysis of PBC subject to the independent cases of pre-strain given by \bar{v}^{kl}_{po} .

In order to derive the sensitivities with respect to the elasticity properties of the macro-material, the local material of an element within PBC can be treated to be isotropic and its Young's modulus can be interpolated as the function of the element density as:

$$E(x_i) = E_1 x_i^p \tag{3}$$

where E_1 denotes the Young's modulus for solid element, p is the penalty exponent and x_i denotes the relative density of the ith element. This material model is often called as "solid isotropic material with penalization" (SIMP) model [4,6]. The penalty exponent p > 1 is artificially applied to make sure that the solution indeed converges to a solid/void design.

With the help of the above material interpolation scheme, the sensitivity of the homogenized elasticity tensor on the design variable, x_0 , can be derived from the adjoint variable method [26], as:

$$\frac{\partial E^{H}_{ijkl}}{\partial x_{i}} = \frac{1}{|Y|} \int_{\Omega} \frac{\partial E_{pqrs}}{\partial x_{i}} \left(\bar{\varepsilon}^{kl}_{pq} - \tilde{\varepsilon}^{kl}_{pq} \right) \left(\bar{\varepsilon}^{ij}_{rs} - \tilde{\varepsilon}^{ij}_{rs} \right) d\Omega \tag{4}$$

where |Y| denotes the total volume of PBC. Substituting Eq. (3) into Eq. (4), the sensitivity of the homogenized elasticity tensor can be re-written as:

$$\frac{\partial E^{H}_{ijkl}}{\partial x_{i}} = \frac{p}{|Y|} \int_{\Omega} x_{i}^{p-1} E^{1}_{pqrs} \left(\bar{\varepsilon}^{kl}_{pq} - \tilde{\varepsilon}^{kl}_{pq} \right) \left(\bar{\varepsilon}^{ij}_{rs} - \tilde{\varepsilon}^{ij}_{rs} \right) d\Omega \tag{5}$$

where E_{nars}^1 is the elasticity tensor of the solid.

3. Optimization problem and BESO sensitivity number

The stiffness of an isotropic elastic material can be described by two moduli, i.e. the bulk modulus K and shear modulus G. To design the stiffest cellular material, the optimization problem can be described as properly distributing the solid material within PBC subject to a given material volume so that the effective bulk or shear modulus approaches its possible maximum value. Thus, the optimization problem can be mathematically stated as follows:

Maximize:
$$K$$
 or G
Subject to: $V^* - \sum_{i=1}^{N} V_i x_i = 0$ $x_i = x_{\min}$ or 1

where V_i is the volume of an individual element and V^* is the prescribed total structural volume. N is the total number of elements in PBC. The binary design variable x_i denotes the density of ith element. To avoid the singularity of the stiffness matrix, a small value of x_{\min} , e.g. 0.001, is used to represent the void elements.

The bulk modulus of the cellular material can be expressed in terms of the components of the effective elasticity tensor E_{ijkl}^H in 2D cases as:

$$K = \frac{1}{4}(E_{1111} + E_{1122} + E_{2211} + E_{2222}) \tag{7}$$

and in 3D cases as:

$$K = \frac{1}{9}(E_{1111} + E_{1122} + E_{1133} + E_{2211} + E_{2222} + E_{2233} + E_{3311} + E_{3322} + E_{3333})$$
(8)

The shear modulus relates the material response to the shear strain and can be expressed in 2D cases as:

$$G = E_{1212}$$
 (9)

and in 3D cases as:

$$G = \frac{1}{3}(E_{2323} + E_{3131} + E_{1212}) \tag{10}$$

As only orthotropic cellular material with square symmetry will be considered in this paper, the following relationships exist: $E_{1111} = E_{2222}$ and $E_{1122} = E_{2211}$ in 2D cases and $E_{1111} = E_{2222} = E_{3333}$, $E_{1122} = E_{2211} = E_{2233} = E_{3322} = E_{3311} = E_{1133}$ and $E_{2323} = E_{3131} = E_{1212}$ in 3D cases.

Similarly, the sensitivity of bulk modulus, $\frac{\partial K}{\partial x_i}$ and shear modulus, $\frac{\partial G}{\partial x_i}$ can be easily calculated with the sensitivities of the effective elasticity tensor in Eq. (5). The sensitivity number in BESO which denotes the relative ranking of all elemental sensitivities can be defined for maximizing the bulk modulus as:

$$\alpha_i = \frac{1}{p} \frac{\partial K}{\partial x_i} \tag{11}$$

and for maximizing the shear modulus as:

$$\alpha_i = \frac{1}{p} \frac{\partial G}{\partial x_i} \tag{12}$$

The sensitivity numbers in Eqs. (11) and (12) indicates the variation of the objective function (K or G) with the design variables, x_i . To maximize the corresponding objective function, the elements

with the higher sensitivity numbers should have x_i increased and elements with lower sensitivity numbers should have x_i decreased. For the BESO method, as the design variables are restricted to be either x_{\min} or 1, the optimality criterion can be described as that sensitivity numbers of solid elements ($x_i = 1$) are always higher than those of void elements ($x_i = x_{\min}$) [21]. Therefore, we devise an update scheme for the design variable x_i by changing from it 1 to x_{\min} for elements with the lowest sensitivity numbers and from x_{\min} to 1 for elements with the highest sensitivity numbers.

4. Numerical implementation and BESO procedure

Topology optimization usually encounters checkerboard patterns and mesh-dependency problems when the design domain is discretized into a large number of low-order elements. To circumvent those problems, we use a mesh-independency filter by averaging the elemental sensitivity number with its neighbouring elements based on image-process techniques [21,22]. The mesh-independency filter works as a low-pass filter that eliminates features below a certain length-scale in the optimal topologies. The elemental sensitivity number will be modified by the following equation:

$$\hat{\alpha}_i = \frac{\sum_{j=1}^N w(r_{ij})\alpha_e}{\sum_{j=1}^M w(r_{ij})} \tag{13}$$

where r_{ij} denotes the distance between the centre of the element i and element j. $w(r_{ij})$ is weight factor is given as:

$$w(r_{ij}) = \begin{cases} r_{\min} - r_{ij} & \text{for } r_{ij} < r_{\min} \\ 0 & \text{for } r_{ij} \geqslant r_{\min} \end{cases}$$
 (14)

where r_{\min} is the filter radius.

In the BESO algorithm, only two discrete design variables x_{\min} and 1 are used. It is almost impossible to obtain a convergent solution especially when a coarse mesh is used. To improve the convergence of the solution, Huang and Xie [22] proposed that the elemental sensitivity number can be further modified by averaging with its historical information, i.e. the sensitivity number after the first iteration is calculated by:

$$\tilde{\alpha}_i = \frac{1}{2}(\hat{\alpha}_{i,k} + \hat{\alpha}_{i,k-1}) \tag{15}$$

where k is the current iteration number. Then let $\hat{\alpha}_{i,k} = \tilde{\alpha}_i$ which will be used for the next iteration, thus the modified sensitivity number considers the sensitivity information in the previous iterations. This algorithm suppresses the changes of design variables for solid ele-

ments with higher historical sensitivity numbers and void elements with lower historical sensitivity numbers, and greatly stabilizes the whole evolution process.

The whole BESO procedure for cellular material design is outlined as follows:

Step 1: Define the BESO parameters with objective volume, V^* , evolutionary ratio ER (normally ER = 0.02), filter radius r_{\min} and penalty factor p (normally p = 3).

Step 2: Discretize the PBC domain using a finite element mesh and construct an initial design. In this paper, the initial designs for 2D and 3D cases are shown in Fig. 1.

Step 3: Apply periodic boundaries on PBC and initial strain loads, \bar{e}_{pq}^{kl} . Carry out finite element analysis (FEA) and output the corresponding strain fields, \tilde{e}_{pq}^{kl} .

Step 4: Calculate the elemental sensitivity numbers α_i according to Eqs. (5), (11), and (12).

Step 5: Filter sensitivity numbers in the PBC domain as Eqs. (13) and (14), and then average with its historical information as Eq. (15).

Step 6: Determine the target volume for the next design. When the current volume V_i is larger than the objective volume V^* , the target volume for the next design can be calculated by:

$$V_{i+1} = V_i(1 - ER) (16)$$

If the calculated volume for the next design is less than the objective volume V^* , the target volume for the next design V_{i+1} is set to be V^* .

Step 7: Reset the design variables of all elements. For solid elements, the elemental density is changed from 1 to x_{min} if the following criterion is satisfied.

$$\alpha_i < \alpha_{th}$$
 (17a)

For void elements, the elemental density is changed from x_{\min} to 1 if the following criterion is satisfied.

$$\alpha_i \geqslant \alpha_{th}$$
 (17b)

where α_{th} is the threshold of the sensitivity number which is determined by the target material volume, V_{i+1} , and the relative ranking of the sensitivity numbers. For example, there are 100 elements in design domain and $\alpha_1 > \alpha_2 \cdots > \alpha_{100}$ and if V_{i+1} corresponds to a design with 70 elements then $\alpha_{th} = \alpha_{70}$.

Step 8: Repeat 3–7 until both the volume constraint and convergent criterion are satisfied. The convergence criterion is

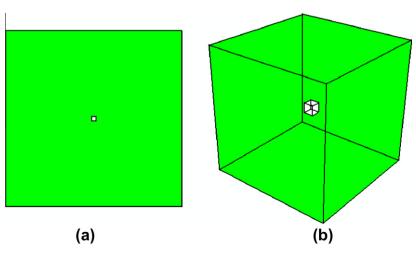


Fig. 1. Initial design (a) 2D cases; (b) 3D cases.

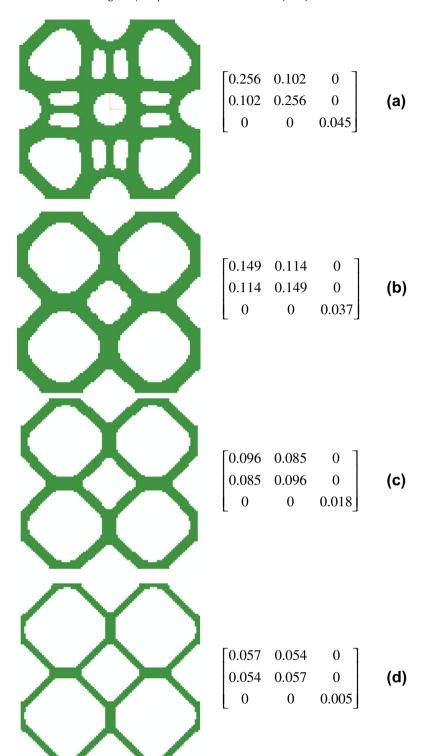


Fig. 2. Microstructures and effective elasticity matrixes of 2D cellular materials with maximum bulk modulus for various volume constraints (a) 50%; (b) 40%; (c) 30% and (d) 20%.

defined in terms of the change in the objective function (K or G)

$$\frac{\left|\frac{\sum_{i=1}^{N} (C_{k-i+1} - C_{k-N-i+1})}{\sum_{i=1}^{N} C_{k-i+1}}\right| \leqslant \tau \tag{18}$$

where *C* is the objective function, *k* is the current iteration number, τ is a allowable convergence error and *N* is integral number. τ and *N*

are set to be 0.1% and 5 respectively throughout this paper. This implies that the change of the objective function over the last 10 iterations is acceptably small (0.1%).

It can be seen that the BESO procedure is very simple without any complex mathematics. As mentioned in the introduction, it can be easily programmed with commercial FEA software packages like ABAQUS as in this paper.

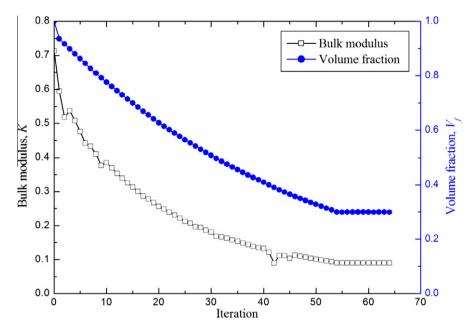


Fig. 3. Evolution histories of bulk modulus, volume fraction and microstructures for maximizing bulk modulus.

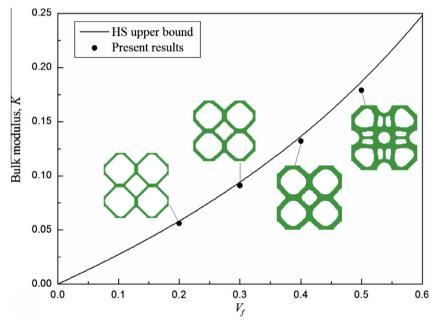


Fig. 4. Comparison between the current solutions and HS upper bound.

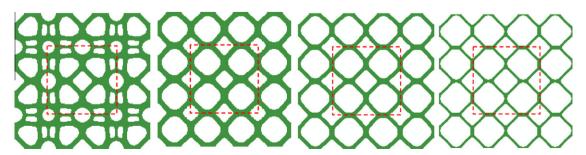


Fig. 5. 2 × 2 base cells with maximum bulk modulus for various volume constraints (a) 50%; (b) 40%; (c) 30% and (d) 20%.

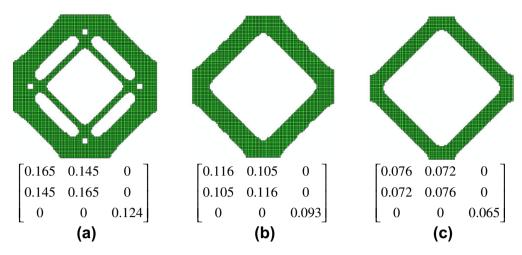


Fig. 6. Microstructures and effective elasticity matrixes of 2D cellular materials with maximum shear modulus for various volume constraints (a) 45%; (b) 35%; and (c) 25%.

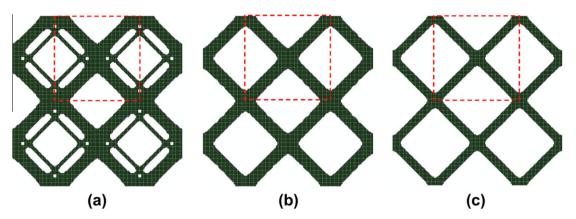


Fig. 7. 2×2 base cells with maximum shear modulus for various volume constraints (a) 45%; (b) 35% and (c) 25%.

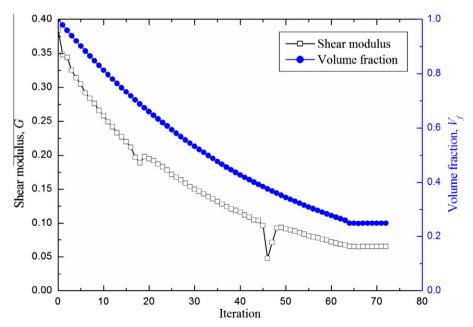


Fig. 8. Evolution histories of shear modulus, volume fraction and microstructures for maximizing shear modulus.

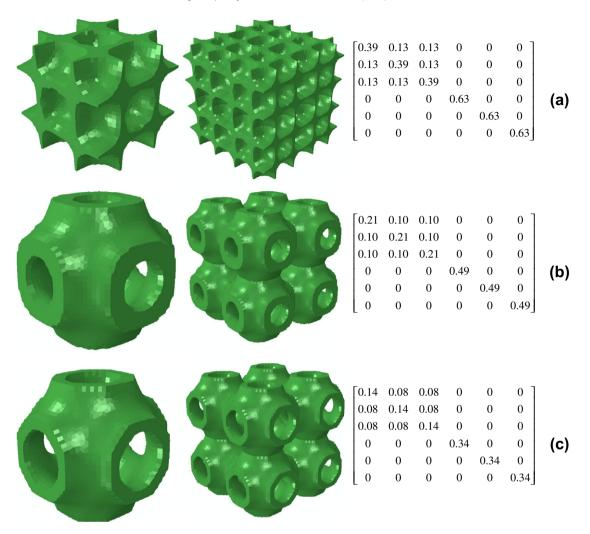


Fig. 9. 3D base cells, $2 \times 2 \times 2$ cells and effective elasticity matrixes of 3D cellular materials with maximum bulk modulus (a) volume fraction is 50%; (b) volume fraction is 40%; and (c) volume fraction is 30%.

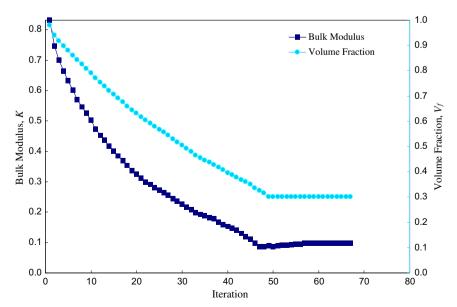


Fig. 10. Evolution histories of bulk modulus, volume fraction and microstructures for maximizing bulk modulus of 3D cellular material.

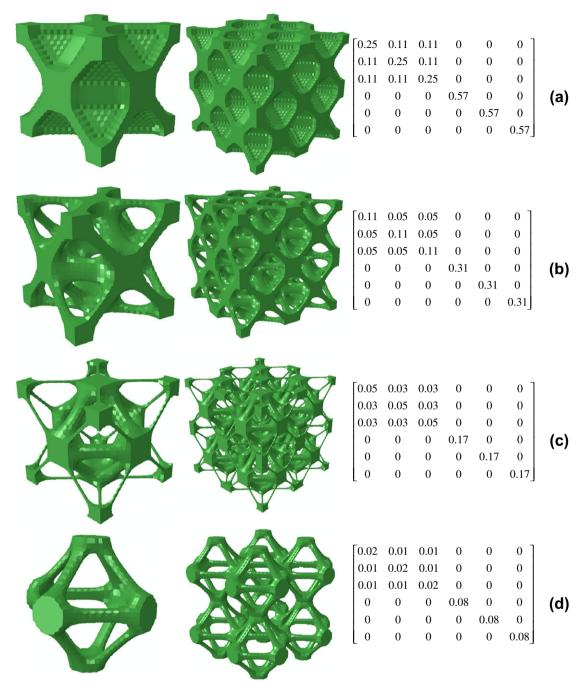


Fig. 11. 3D base cells, $2 \times 2 \times 2$ cells and effective elasticity matrixes of 3D cellular materials with maximum shear modulus (a) volume fraction is 40%; (b) volume fraction is 30%; (c) volume fraction is 20%; (d) volume fraction is 10%.

5. Examples and discussion

5.1. 2D examples for maximizing the bulk modulus

In this section, the square design domain with dimensions 100×100 is discretized into 100×100 4-node quadrilateral elements. Young's modulus and Poisson's ratio of solid material are selected as E=1 and v=0.3 respectively. The other parameters are set up as evolution rate ER=0.02, filter radius $r_{\min}=5$ and penalty exponent p=3. The BESO procedure starts from an initial guess design as shown in Fig. 1a which assigns four soft elements at the centre of the design domain. When the volume constraints of solid material are set to be 50%, 40%, 30% and 20% of the design

domain respectively, the corresponding final microstructures and their effective elasticity matrixes are given in Fig. 2. The total iterations for the corresponding cases are 49, 56, 64 and 80. The bulk moduli of these microstructures are 0.179, 0.132, 0.091 and 0.056 respectively.

Fig. 3 shows the evolution histories of bulk modulus and volume fraction as the volume constraint of solid material is 30%. Generally, the bulk modulus decreases as the total volume of the solid decreases. Once the volume constraint is satisfied, the objective function (bulk modulus) and micro-structural topologies stably converge to their final solutions. The final microstructure of cellular material as shown in Fig. 2c can be interpreted as four octagonal honeycomb cells whose bulk modulus equals to one

octagonal honeycomb cell in Sigmund [12] using a truss modelled base cell.

Neves et al. [14] has identified that the maximum bulk modulus of orthotropic material with square symmetry approaches to the Hashin–Strickman (HS) upper bound [27]. The HS bound is used for predicting the range of properties that a composite could achieve with given material composition and volume fractions. In the limit when the properties of one of the phases (voids) are equal to zero, the HS upper bound can be defined as [28]:

$$K_{upper} = \frac{V_f KG}{(1 - V_f)K + G} \tag{19}$$

where K and G are the bulk and shear moduli of the solid, V_f is the volume fraction of the solid material. Replotting the bulk modulus of the above microstructures in Fig. 4 indicates that the present solutions are indeed close to the HS upper bound in Eq. (19). It also verifies the effectiveness of the current BESO procedure for finding a microstructure with the maximum bulk modulus.

The macrostructures of the cellular material can be constructed periodically by the above microstructures as depicted by Fig. 5 with 2×2 base cells. It is obvious that the bulk modulus of the 2×2 base cells equals to that of their single base cells. Therefore, this 2×2 base cells are also the solutions for the current problem. Meanwhile, one may start BESO from an initial design with a soft element at the four corners of the design domain, the expected micro-structural topologies should be those inside square boxes shown in Fig. 5. It can be seen that there are a number of equivalent solutions having the maximum bulk modulus and the microstructure obtained highly depends on initial design and other optimization parameters and algorithm as well.

5.2. 2D examples for maximizing shear modulus

The same design domain as in the above example is also discretized into 100×100 4-node quadrilateral elements. Young's modulus and Poisson's ratio of solids are E=1 and v=0.3. The objective of the following examples is to find microstructures with maximum shear modulus for various material volume constraints. The BESO parameters are ER=0.02, $r_{\min}=5$ and p=3.

BESO starts from the initial design as shown in Fig. 1(a). Convergent solutions are obtained after 48, 59 and 73 iterations when the volume fractions of solids are 45%, 35% and 25% respectively. The final microstructures and effective elasticity matrixes are shown in Fig. 6 and their shear moduli are 0.124, 0.093 and 0.065. To show the macrostructure of the material and possible solution from another initial design, the 2×2 base cells are constructed periodically as shown in Fig. 7. As explained above, this 2×2 base cells have the same shear moduli as that of their original base cell. As BESO starts from the initial design with four soft elements at the centre of sides, one can obtain the micro-structural topologies inside the square boxes in Fig. 7. These diamond microstructures are the same as the solutions in Neves et al. [14]. Fig. 8 shows the evolution histories of shear modulus and volume fraction for V_f = 0.25. It is also demonstrated that shear modulus stably converges after the volume constraint is satisfied.

5.3. 3D examples for maximizing bulk modulus

The cubic domain with dimensions $26 \times 26 \times 26$ is discretized with $26 \times 26 \times 26$ 8-node brick elements. The mechanical properties of solids are Young's modulus E=1 and Poisson's ratio v=0.3. The BESO parameters are ER=0.02, $r_{\min}=3$ and p=3. BESO starts from the initial design shown in Fig. 1b where eight elements at the centre are assigned as soft elements.

The objective is to find a 3D micro-structural topology with the maximum bulk modulus K for a given volume constraint. The obtained topologies of the base cells and $2 \times 2 \times 2$ base cells are shown in Fig. 9 as the volume constraints of solids are set to be 50%, 40% and 30% of the design domain respectively. The total iterations are 51, 71 and 66 and the bulk moduli are 0.218, 0.139 and 0.098. Fig. 10 shows the evolution histories of bulk modulus and volume fraction during iterations for the volume constraint $V_f = 0.3$.

5.4. 3D examples for maximizing shear modulus

The cubic domain with dimensions $26 \times 26 \times 26$ is discretized with $26 \times 26 \times 26$ 8-node brick elements. The mechanical properties of solids are Young's modulus E = 1 and Poisson's ratio v = 0.3. The BESO parameters are ER = 0.02, $r_{\min} = 1.5$ and p = 3. Here a small filter radius is used in order to have some thin members in the final micro-structural topology. BESO still starts from the initial design shown in Fig. 1b. The volume constraints of solids are set to be 40%, 30%, 20% and 10% of the whole design domain, respectively.

Fig. 11 shows the obtained micro-structural topologies of the base cell, and their $2\times2\times2$ base cells and effective elasticity matrixes for various volume constraints. The total iterations are 49, 90, 88 and 111 and the final shear moduli are 0.567, 0.307, 0.171 and 0.084. The base cell for 10% volume constraint clearly gives an octahedron cell.

6. Conclusion

This paper has developed a new approach to designing microstructures of cellular materials with maximum bulk or shear modulus based on the BESO technique. The BESO algorithm seeks optimal material distribution within the periodic base cell by performing topology optimization subject to a volume constraint. The effective elasticity matrix is homogenized within PBC and elemental sensitivity numbers are established to measure the change of the bulk or shear modulus due to the variation of the elemental density. According to the elemental sensitivity numbers, BESO changes the density of elements from 1 to x_{\min} or from x_{\min} to 1 iteratively until the solution converges. Several 2D and 3D examples are presented to demonstrate the effectiveness of the proposed BESO method. Some interesting topological patterns have been found for guiding the cellular material design.

Acknowledgement

This research is supported by the Australian Research Council under its Discovery Projects funding scheme (Project No. DP1094403).

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