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The Design of Functional Gradient Materials with Inverse Homogenization method

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Abstract. This study systemically presents an inverse homogenization method in the design of functional gradient materials, which gained substantial attention recently due to their layer-by-layer defined physical properties. Each layer of these materials is unilaterally constructed by periodically extended microstructural elements (namely base cells), whose effective properties can be decided by the homogenization theory in accordance with the material distribution within the base cell. The design objective is to minimize the summation of the least squares of the difference between corresponded entries in target and effective elasticity tensors. The method of moving asymptote drives the minimization of this positive objective function, which forces the effective values approach to the targets as closely as possible. The sensitivity of the effective elasticity tensors with respect to the design variables is derived from the adjoint variable method and it guides the minimization algorithm efficiently. To guarantee the connectivity between adjacent layers, non-design domains occupied by solid materials acting as connective bars are fixed in the design of base cells. Furthermore, nonlinear diffusion technique is introduced to avoid checkerboard patterns and blur boundaries in the microstructures. A series of two-dimensional examples targeted for the elasticity tensors with same extreme Poisson ratios but different densities in each layer are illustrated to highlight the computational material design procedure.

Introduction

The physical properties of functionally graded materials (FGMs) vary gradually in given direction in terms of the functional requirements. Such extraordinary properties attract many material engineers and scientists to the design and fabrication of artificial FGMs during the last two decades. Being a relatively new computational technique, the inverse homogenization method [1] signifies a novel material design paradigm. This method is rooted in topology optimization algorithms [2] with a primary focus on microstructural material design of a base cell model. By properly allocating solid materials, the desirable homogenized material properties like Poisson ratios can be attained. However, the existing version of inverse homogenization procedure is restricted in generating macrostructurally homogeneous periodic composite without involving gradient effective properties. This paper attempts to extend the classical material design to FGM for accommodating desirable gradient mechanical properties in a multiply-layered fashion.

To briefly describe the design idea, a base cell with periodic boundary conditions is used to seek the optimal material distribution for a specific effective property. Then a layer of the material is constructed by periodically extending the base cells along the direction perpendicular to the property gradient. Finally, the FGM structure is materialized by assembling layer-by-layer along the desired gradient direction. The effective property for each layer can be calculated by the finite element based homogenization algorithm [3] within its base cell. In this study, the design objective is to minimize the summation of the least squares of the difference between corresponded entries in target and effective elasticity tensors. To enable an appropriate connection between adjacent layers, non-design domains occupied by solid materials are imposed in the design. A nonlinear diffusion technique [4] is adopted to avoid checkerboard patterns and blur boundaries of the microstructure. The adjoint variable method [5] is used to obtain the sensitivity of the objective function with respect to topological variables (i.e. relative density). The minimization of this positive objective function is performed by the method of moving asymptote (MMA) [6]. The numerical experiments provide a series of novel gradient microstructures with specified gradient property.

Statement of the problem and the design methodology

Based on the homogenization theory [3], any point in a two-phase (solid-void) composite is not continuum but a microstructure with some special shape and topology. If the architectures of such microstructures regularly vary in a given direction under the requirements of some special property criterions, then the composite is named as the functionally graded materials. The local density $\rho(\mathbf{x})$ within microstructural base cell is used as the design variable to represent the solid phase ($\rho(\mathbf{x})$=1) and void phase ($\rho(\mathbf{x})$=0), respectively. As widely described in density-based structural topology optimization, the design variable is usually relaxed from 0/1 to intermediate values between 0 and 1 and be penalized as $\rho(\mathbf{x})^p$ in terms of the "solid isotropic material with penalization" (SIMP) [7].

The homogenization theory [3] defines the effective elasticity tensor for a microstructure occupying volume Ω as,

$$\bar{D}_{ijkl}(\rho) = \frac{1}{|\Omega|}\int_{\Omega} D_{ijmn}(\rho)\left(\bar{\varepsilon}^{kl}_{mn} - \tilde{\varepsilon}^{kl}_{mn}\right)d\mathbf{x} \tag{1}$$

where $\bar{\varepsilon}^{kl}_{mn}$ are the linearly independent unit test strain fields given as $\bar{\varepsilon}^{11}_{mn} = \begin{pmatrix}1 & 0 & 0 & 0\end{pmatrix}^T$, $\bar{\varepsilon}^{22}_{mn} = \begin{pmatrix}0 & 1 & 0 & 0\end{pmatrix}^T$, $\bar{\varepsilon}^{12}_{mn} = \begin{pmatrix}0 & 0 & 1 & 0\end{pmatrix}^T$ and $\bar{\varepsilon}^{21}_{mn} = \begin{pmatrix}0 & 0 & 0 & 1\end{pmatrix}^T$ separately. The local elasticity tensor is denoted as $D_{ijmn}(\rho)$. The strain fields $\tilde{\varepsilon}^{kl}_{mn}$ induced from the test strains are the solutions to the following equation

$$\int_{\Omega} D_{ijmn}\varepsilon_{ij}(\mathbf{\upsilon})\tilde{\varepsilon}^{kl}_{mn}d\mathbf{x} = \int_{\Omega} D_{ijmn}\varepsilon_{ij}(\mathbf{\upsilon})\bar{\varepsilon}^{kl}_{mn}d\mathbf{x} \tag{2}$$

where the virtual displacement field $\mathbf{\upsilon} \in H_{per}$ belongs to the periodic Soblev functional space. To avoid the checkerboard pattern and blur boundaries (too many intermediate values), restriction to the norm of the gradient of the design variable ($\|\nabla\rho\|$) with the nonlinear diffusion technique [4] is considered, leading to the objective function,

$$\min_{\rho} J(\rho) = \sum_{i,j,k,l=1}^{4} \frac{1}{2} r_{ijkl}\left(\overset{*}{D}_{ijkl} - \bar{D}_{ijkl}\right)^2 + \varepsilon^2\varphi\left(\|\nabla\rho\|\right) \tag{3}$$

where r_{ijkl} and ε are positive factors to control the role of different entries in target elasticity tensor $\overset{*}{D}_{ijkl}$ and the nonlinear diffusion. Without a doubt, imposing feasible connection zones in the topological design can be a critical step since they usually lead to different final shapes and topologies for the base cells. As the MMA method [6] is used for minimizing the objective function, we have to derive the sensitivity of the objective function with respect to the design variable by,

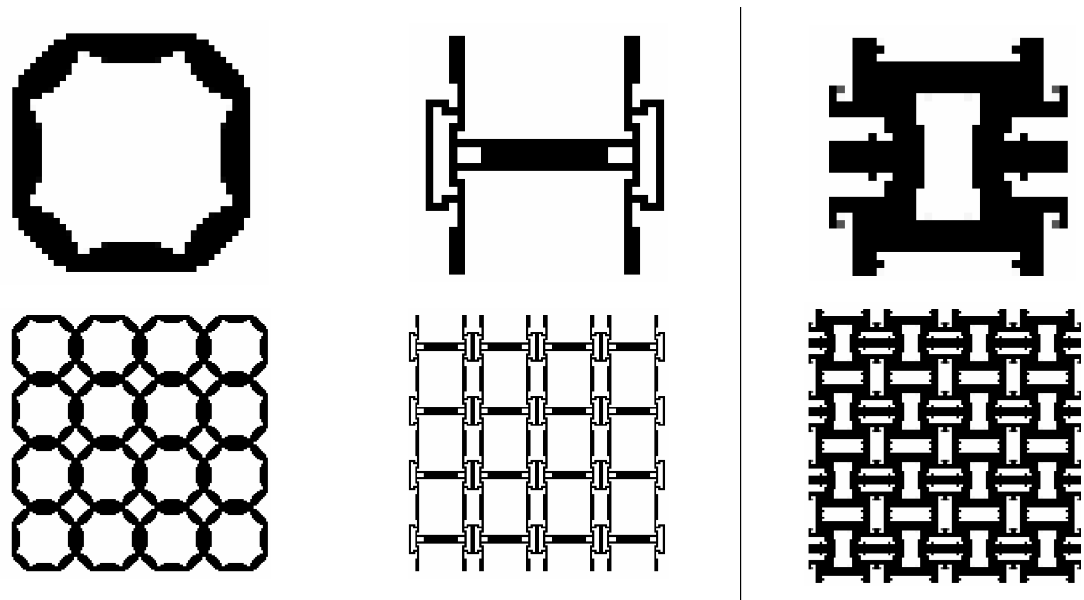
$$\frac{\partial J}{\partial \rho} = -\sum_{i,j,k,l=1}^{4} r_{ijkl}\left(\overset{*}{D}_{ijkl} - \tilde{D}_{ijkl}\right)\frac{\partial \tilde{D}_{ijkl}}{\partial \rho} - \varepsilon^2 div\left(\frac{\varphi'\left(\|\nabla\rho\|\right)}{\|\nabla\rho\|}\nabla\rho\right) \tag{4}$$

where $\partial D_{ijkl} / \partial \rho$ can be derived from the adjoint variable method [5] as

$$\frac{\partial}{\partial \rho}\tilde{D}_{ijkl}\left(\rho\right) = \frac{1}{|\Omega|}\int_{\Omega}\left(\bar{\varepsilon}_{mn}^{kl} - \tilde{\varepsilon}_{mn}^{kl}\right)\frac{\partial D_{ijmn}\left(\rho\right)}{\partial \rho}\left(\bar{\varepsilon}_{mn}^{kl} - \tilde{\varepsilon}_{mn}^{kl}\right)d\mathbf{x} \tag{5}$$

Results and discussion

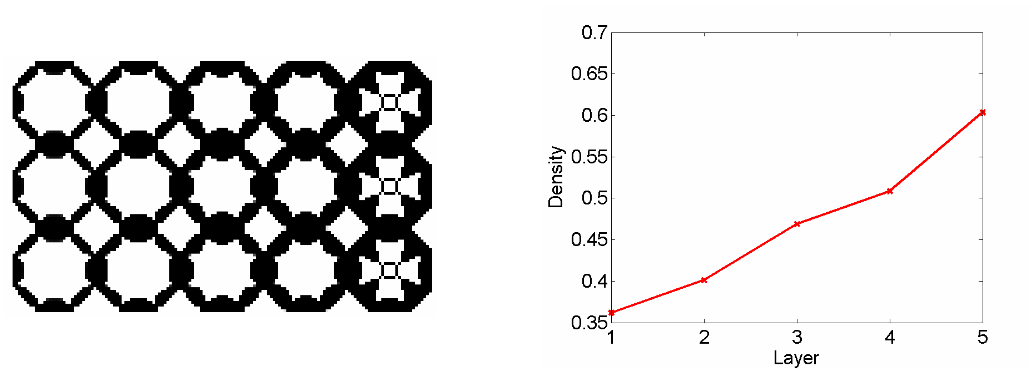
In the microstructural topology optimization, two initial values of material distributions are typically used. The first involves an initial material distribution, where the pixel (element) density (volume fraction) is proportional to the distance between the pixel center and the center of the base cell. The second one involves a pattern whose elemental density is inversely proportional to this distance. For the former, the high density materials extend from boundary to the inner area in the radial direction. One benefit of using this initial distribution is that the connection constraints may not be required since the more often than not the dense boundary materials are not relocated completely, thereby enabling boundary connection. But for the second initial value, certain connection across the property-gradient direction must be taken into account as the materials spread from center to boundary leading to topological breakage across the shared border of two graded base cells, which yields meaningless functionally graded materials. Before illustrating the FGM examples, we provide two benchmarking examples for the composites with extreme positive (v=1; top figures in Fig.1 a) and negative Poisson rations (v= –1 top figures in Fig.1 b and c), respectively. The bottom figures in Fig. 1 are the assembly of the composites composed by periodically repeated base cells for these examples.



(a) (b) (c)

Fig. 1. Base cells and their ranked microstructures (4×4) with: (a) Poisson's ratio v=1; (b) Poisson's ratio v= –1 (case 1); (c) Poisson's ratio v= –1 (case 2).

Fig. 2 (a) illustrates the FGM with same positive Poisson's ratio but different density in each layer (shown as in Fig. 2 (b)). This example starts from the first initial value and don't need to set the fixed non-design domains along the boundary. Fig. 3 gives the FGM with same negative Poisson ratio but different density in each layer. As the second initial value is applied, the fixed non-design domains (red regions in Fig. 3) are set during the design. It has to note here that sometimes the fixed non-design domains are necessary even starting from the first initial value in the case that the numerical implementation is unstable.



(a) (b)

Fig. 2. Design of FGM with positive Poisson's ratio (v=1) but different densities in each layer: (a) FGM microstructures; (b) Density in each layer.

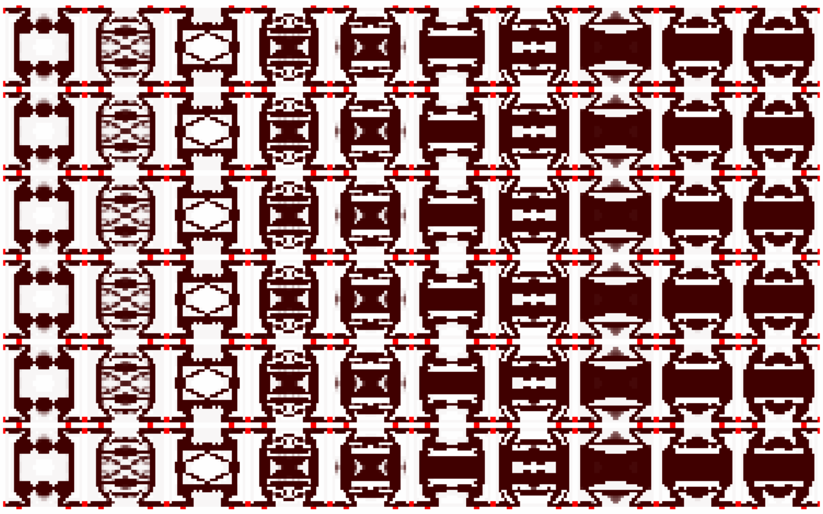


Fig. 3. Design of FGM with negative Poisson's ratio (v=–1) but different densities in each layer

Conclusions

This paper presented a simple but useful method in the FGM design. With the introduction of nonlinear diffusion technique, the boundaries of the optimal microstructures are edge-preserving and checkerboard-free. On the other hand, fixed non-design domain guarantees the correct connection between adjacent layers.

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