Computational Materials Science 82 (2014) 457–463

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Maximizing stiffness of functionally graded materials with prescribed variation of thermal conductivity

A. Radman [a], X. Huang [a,b,*], Y.M. Xie [a]

[a] Centre for Innovative Structures and Materials, School of Civil, Environmental and Chemical Engineering, RMIT University, GPO Box 2476, Melbourne 3001, Australia
[b] Department of Building Engineering, Tongji University, Shanghai 200092, China

ARTICLE INFO

Article history:
Received 12 August 2013
Received in revised form 1 October 2013
Accepted 13 October 2013
Available online 12 October 2013

Keywords:
Topology optimization
Functionally graded material
Bulk modulus
Thermal conductivity

ABSTRACT

This paper presents a computational technique for the topological design of microstructures for functionally graded materials (FGMs) with multiple graded properties of bulk modulus and thermal conductivity. The inverse homogenization method is applied for the design of a series of base cells with two constituent materials. The topology optimization of microstructures is performed by using the bi-directional evolutionary structural optimization (BESO) method, which imposes a constraint on the effective thermal conductivity. A computationally efficient approach is developed to provide smooth transition between cells by considering three cells at each stage of the optimization. Numerical examples are presented to demonstrate the effectiveness of the algorithm. The proposed approach could also be used for the design of FGMs with other functional properties.

1. Introduction

From previously published works on stress distribution on woody stem of trees (e.g. [1]), it has become evident that biological materials achieve different properties through changes in their hierarchical structures in order to adapt to the environmental stimuli [2]. However, it was not until 1972 when the industrial benefits of materials with graded functional properties was first analytically discussed by published papers of Shen and Bever [3] and Bever and Duwez [4] in 1972. The idea did not receive much attention until mid-1980s when the manufacturing technologies allowed the concept to be practically used for industrial applications. The morphology of primary invented functional graded material (FGM) consists of embedment of a ceramic phase into a steel phase with varying volume fractions thereby enabling the gradation in properties along certain directions. The ceramic phase acts as a thermal barrier, protecting the metallic phase from corrosion and oxidation and the metallic phase strengthens the composite; hence, demonstrating a multi-functional characteristics within the thickness of the composite [5].

For materials made of periodic base cells (PBC) the "inverse homogenization" approach has been introduced by Sigmund [6,7], which enables topology optimization of the microstructures for materials with the goal of materials properties at macro-scale to be improved or tailored for specific functions. Inspired by the approach, some attempts have been made for development of multi-functional materials such as materials with prescribed combinations of stiffness and thermal conductivity [8], heat and electricity transport [9], stiffness and permeability [10] and other multi-physical properties [11–13].

The common approach in the design of materials with multi-functional characteristics is to minimize (or maximize) a linear combination of functional properties [12]. Assuming two functional properties of f_1 and f_2 for the composite, the optimization objective function is usually defined by applying some weighting factors to different parts of the objective functions. By varying the weighting factors, materials with multiple properties could be achieved due to the competence of two properties [9,10,12,14]. However, a drawback of such an approach is that the equidistant changes in weighting factors do not guarantee the same variations in physical properties of the designed material [14]. Apart from the non-linear cross properties of the defined objective functions, the reason largely attributes to the existence of many local optima which may cause the algorithms to be unable to avoid a nearby solution. Therefore, the results are usually expressed as a generated Pareto front [13–15] which enables a visual representation of attainable functional properties with respect to the weighting factors for a particular setting of design parameters. Consequently, this optimization approach with given weighting factors, is not appropriate for the design of FGMs for a prescribed gradient because of the uncontrolled fluctuations of properties of the generated microstructure.

In the traditional design approach of FGMs, the gradient of a property was realized by gradually varying the volume fractions of their constituents [16,17]. The systematic design methods of

* Corresponding author. Tel.: +61 3 99253320; fax: +61 3 96390138.
E-mail address: huang.xiaodong@rmit.edu.au (X. Huang).

0927-0256/$ - see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.commatsci.2013.10.024

FGMs, utilizing topology optimization techniques have been introduced by Zhou and Li [18,19] and Radman et al. [20]. In those studies, the microstructures of cellular FGMs was represented with a series of base cells. Topology optimizaiton aims to find the optimal topologies of these base cells so that the FGMs exihibit the gradual varition of a prescribed property.

In this paper, we present a computational technique for the topological design of microstructures for FGMs with two constituent phases which possess multiple graded properties, e.g. bulk modulus and thermal conductivity. It is assumed that the FGM is composed of a series of base cells and the topology optimization problem is solved by utilizing the BESO structural topology optimization technique [21,22]. Instead of assigning fixed weight factors to different terms of objective function, an optimization problem statement is defined to maximize one functional property with the constraint on the gradual change of another functional property. To improve the connectivity of adjacent base cells, they are optimized progressively by considering three base cells at each stage. Numerical examples show that the approach yields the accurate control of the constraint value and improves the connectivity of neighboring cells in a more computationally efficient manner.

2. Topology optimization

2.1. Problem statement

By assuming N base cells along the gradation direction of the FGM as illustrated in Fig. 1, the topology optimization problem for obtaining materials with maximum stiffness and prescribes gradation of thermal conductivity and volume fraction can mathematically be defined for the jth PBC as:

$$\text{Maximize}: \quad K^j \tag{1a}$$

$$\text{Subject to}: \quad k_c^j = k_c^{j*} \tag{1b}$$

$$V^j = \sum_{i=1}^{M} x_i^j V_i^j \qquad x_i^j = x_{\min} \text{ or } 1 \tag{1c}$$

$$(i = 1, 2, \cdots, M) \text{ and } (j = 1, 2, \cdots, N)$$

where M is the total number of finite elements within each base cell. It is assumed that the base cells are composed of two constituent materials with Young's modulus and thermal conductivity of E^1 and K^1 for material 1 and E^2 and K^2 for material 2; V^j denotes the volume (or weight) of material 1 in the jth base cell; K^j is the bulk modulus of the jth base cell; k_c^j and k_c^{j*} are the effective thermal conductivity and its prescribed value of the jth base cell respectively.

The design variable x_i^j of the ith element within the jth base cell can take a binary value of either 1 for elements with material 1 or a small value (i.e. $x_i = 0.001$) for elements with material 2. The local material of an element within the PBC is assumed to be isotropic, with the physical property that varies between the properties of the two constituent phases. For the cases in which the materials have well-ordered properties (i.e. $E^1 > E^2$ and $k^1 > k^2$), the following SIMP [23,24] interpolation scheme is applied

$$D_{ij} = x_i^p D_{ij}^1 + (1 - x_i^p) D_{ij}^2 \tag{2a}$$

$$k_{ij} = x_i^p k_{ij}^1 + (1 - x_i^p) k_{ij}^2 \tag{2b}$$

in which D_{ij} and k_{ij} are the elements of stiffness and thermal conductivity matrices respectively and the superscripts indicate the material numbers; p is the penalty exponent ($p = 3$ is used). When the two constituent phases are ill-ordered, (i.e. $E^1 > E^2$ and $k^1 < k^2$) the interpolation scheme can be defined as:

$$D_{ij} = x_i^p D_{ij}^1 + (1 - x_i^p) D_{ij}^2 \tag{3a}$$

$$\frac{1}{k_{ij}} = \frac{x_i}{k_{ij}^1} + \frac{(1 - x_i)}{k_{ij}^2} \tag{3b}$$

2.2. Homogenization and sensitivity analysis

For the design of materials microstructures, there is a need for calculation of the overall properties of composite materials based on the spatial distribution of constituent phases. For a material with periodic microstructures, its effective (average) property could be calculated by using the homogenization theory [25–27]. For example, the homogenized elasticity matrix $\mathbf{D}^H$ of such materials is expressed as:

$$\mathbf{D}^H(\mathbf{x}, \mathbf{u}) = \frac{1}{|Y|} \int_Y \mathbf{D}(\mathbf{x})(\mathbf{I} - \mathbf{B}\mathbf{u}) dY \tag{4}$$

in which $\mathbf{u}$ denotes the displacement field, resulted from the finite element analysis of the base cell under periodic boundary conditions and equivalent forces that causes uniform unit strains fields (e.g. $\{1, 0, 0\}^T$, $\{0, 1, 0\}^T$ and $\{0, 0, 1\}^T$ in 2D cases) within the base cell; $\mathbf{I}$ is the unit matrix; $|Y|$ is the total area or volume of the base cell and $\mathbf{B}$ is the strain–displacement matrix. The derivation of $\mathbf{D}^H$ with respect to the design variables x_i, can be found by using the adjoint method [22,28] as

$$\frac{\partial \mathbf{D}^H}{\partial x_i} = \frac{1}{|Y|} \int_Y (\mathbf{I} - \mathbf{B}\mathbf{u})^T \frac{\partial \mathbf{D}}{\partial x_i} (\mathbf{I} - \mathbf{B}\mathbf{u}) dY \tag{5}$$

Similarly, the homogenized thermal conductivity matrix ($\mathbf{k}^H$) can be calculated as:

$$\mathbf{k}^H(\mathbf{x}, \boldsymbol{\mu}) = \frac{1}{|Y|} \int_Y \mathbf{k}(\mathbf{x})(\mathbf{I} - \boldsymbol{\mu}) dY \tag{6}$$

in which $\boldsymbol{\mu}$ is the induced temperature field resulting from finite element analysis of the base cell under the periodical boundary conditions and uniform heat flux (e.g. $\{1, 0\}^T$ and $\{0, 1\}^T$ in 2D cases). The sensitivity of the homogenized thermal conductivity with respect to the design variables can be expressed as [26,29]

$$\frac{\partial \mathbf{k}^H}{\partial x_i} = \frac{1}{|Y|} \int_Y (\mathbf{I} - \boldsymbol{\mu})^T \frac{\partial \mathbf{k}}{\partial x_i} (\mathbf{I} - \boldsymbol{\mu}) dY \tag{7}$$

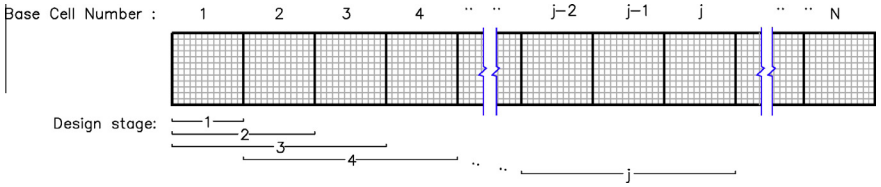

Fig. 1. FGM base cells numbering and design stages.