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Topological design of microstructures of multi-phase materials for maximum stiffness or thermal conductivity

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ABSTRACT

This paper introduces an alternative approach for the topological design of microstructures of materials that are composed of three or more constituent phases. It is assumed that the materials are made up of periodic microstructures. Bi-directional Evolutionary Structural Optimization (BESO) methodology is applied for designing materials' microstructures with maximum bulk modulus, shear modulus or thermal conductivity. Constituent phases are divided into groups and sensitivity analyses are performed in order to estimate their effects on the variation of the objective function. Changing the elemental properties in the finite element model of the microstructure is performed based on this sensitivity analyses and by imposing volume constraints on the constituent phases. Numerical examples are presented to demonstrate the effectiveness of the algorithm in terms of identification of the phases' boundaries and convergence speed. The proposed approach could potentially be used to design multiphase materials for functional properties other than stiffness and thermal conductivity.

1. Introduction

In comparison with cellular materials that are composed of one solid phase and a void phase, composites of two or more materials are more advantageous and attractive for practical applications. One of the reasons is that by combining different constituent phases, a wider range of properties could be achieved which are not attainable by individual constituent phases. In addition, multi-functional multifunctional composites more often than not consist of two or more constituent phases [1].

It is known that the physical properties of composites can be altered by changing the composition and/or microstructural topology of the constituent phases. To find the best spatial distribution of the constituent phases within the microstructure of a composite, structural topology optimization methodology can be applied [2,3]. Here, the aim is to solve the inverse problem of finding microstructures with desired functional properties [2]. Different topology optimization techniques offer advantages and disadvantages in terms of computational cost and efficiency, quality of generated microstructures, robustness, and the level of effort for implementation as a computational post-processing procedure, to name few.

In optimization of microstructures for multi-phase materials, it is desirable to represent the topology of the constituent phases by continuous interface functions. The level-set topology optimization method [4] can provide such sharp interfaces between different constituent phases. For this purpose, the approach requires the definition of higher-dimensional functions to represent the boundaries of constituent phases which is mathematically complicated [5]. In addition special attention must be paid to the splitting of phases. The level-set method is generally devised to describe the propagation of interfaces with a defined speed function; therefore, new phase regions within existing shapes and away from the boundaries cannot be initiated without additional schemes [6,7]. Because of the mathematical complications, in general the approach has not reached the stage of regular application for the design of composites with multiple phases.

Homogenization method [8] has also been used for topology optimization of materials' microstructures in a number of studies [9,10]. In these studies the materials' microstructures are considered as a combination of even much smaller microstructures. These latter microstructures are introduced with different material models such as square unit cells with rectangular void or rank layered materials and their properties are controlled by their geometrical parameters. The geometrical parameters are defined as design variables. The objective of optimization is to find their optimal values (for example the sizes and orientation of the void regions in square unit cells). Except for the issue of existence of solutions [11], these types of topology optimization require performing multi-scale analysis [10] which is costly. In addition, in the case of multiphase materials,

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the generated ranked laminates have zero shear stiffness in one direction, which makes the solutions unstable [12]. Besides, the optimal solutions usually have high manufacturing costs since there are infinitesimal cavities in the microstructures [12].

Inspired by the homogenization method, Solid Isotropic Material with Penalization (SIMP) has been proposed [8]. It has also been tailored for the design of periodic microstructures for composites with two material phases and a void phase [13,14]. The key point in these studies is the introduction of three design variables (x_{i1}, x_{i2}, x_{i3}) for each element that corresponds to three constituent phases. By defining an artificial mixing function, local material properties are correlated with the design variables. This assumption is only valid if the design variables take their extreme values (for example $x_{i1} = 1$ and x_{i2}, $x_{i3} = 0$, which means that the element is filled with constituent phase 1). To circumvent the numerical instabilities associated with utilizing discrete design variables, the SIMP uses a relaxation method in which the design variables are freed to take any value between 0 and 1 [15]. Such an approach leads to intermediate densities in the final topology. In the SIMP approach, it is tried to eliminate the intermediate densities through penalization in the final solution. However, increasing the penalty exponent not only cannot solve the problem completely, but also may result in difficulties in convergence of the solution [16–18]. In comparison with cellular microstructures designed with single material phase, in topology optimization of multi-phase materials the SIMP usually causes more difficulty in interpretation and identification of the boundaries between constituent phases [19]. Several approaches have been proposed to tackle this issue in literature; Heaviside projection algorithm [20], nonlinear diffusion techniques [21] and the phase field approach based on Cahn–Hilliard model [19] are some of the these methods. Nevertheless, these methods add additional computational cost to the optimization procedure.

Recently, the BESO approach has been developed for stiffness optimization of macro-structures with multiple materials [22,23]. Although the generated structures are topologically similar to the results of the SIMP approach, it has been shown that the procedure is independent of the selection of penalization factor and provides clearer boundaries between different materials. Better convergence of the procedure together with high computational efficiency and more importantly, the capability of the BESO in separating the constituent phases, has made it a more promising tool for topology optimization of multi-phase composite structures.

In this paper, the BESO methodology will be extended into the design of composite materials with three or more non-zero constituent phases. It is assumed that the material is composed of periodic base cells (PBC) and the relationship between material's properties at the macroscopic level and microstructure at the microscopic level is established through the homogenization theory [24,25]. The objective function is defined to achieve materials with maximum bulk modulus, shear modulus or thermal conductivity. The constituent phases are categorized into some groups and sensitivity analyses are performed to assess the contribution of elements within each group to the variation of the objective function. The material type of each element is determined based on these sensitivity numbers and by imposing the volume constraints. To tackle the numerical issues, the filtering is conducted within the elements of each group. Finally, some 2D and 3D numerical examples are presented.

2. Methodology

2.1. Problem statement

The stiffness of a composite material can be described by its bulk or shear modulus of elasticity. Similarly thermal conductivity indicates the behavior of materials in transferring heat. In the stiffness optimization problems, it is assumed that the composite material consists of N constituent phases with equal Poisson's ratios and Young's moduli which are ordered descending (that is: $E^1 > E^2 > \ldots > E^N$). Likewise in the conductivity problems, it is assumed that the thermal conductivities of constituent phases are ordered as $\kappa^1 > \kappa^2 > \ldots > \kappa^N$.

Moreover, it is assumed that the microstructure of composites is represented by a PBC which is discretized into finite elements. The optimization problem statement for attaining a periodic microstructure for composite with maximum bulk modulus, shear modulus or thermal conductivity and with constraints on volume fraction of each constituent phase can be expressed as:

$$\text{Maximize} \quad f(x_{ij}) = K, G \text{ or } \kappa_c$$

$$\text{Subject to}: \quad V^{j*} = \sum_{i=1}^{M} x_{ij} V_i - \sum_{m=1}^{j-1} V^{m*} \tag{1}$$

$$x_{ij} = x_{\min} \text{ or } 1$$

where K, G or κ_c are the bulk modulus, shear modulus or thermal conductivity of composite; M is the total number of elements within the finite element model of the PBC; i and j denote the number of the finite element in the PBC and the number of the constituent phase, respectively. V_i and V^{j*} denote the volume of element i and the prescribed volume of the jth constituent phase. x_{ij} is the design variable which indicates the density of the ith element for the jth material phase and is expressed by:

$$x_{ij} = \begin{cases} 1 & \text{if} \quad E \geq E^j \text{ or } (\kappa > \kappa^j) \\ x_{\min} & \text{otherwise} \end{cases} \tag{2}$$

where E and κ denotes the Young's modulus and thermal conductivity of the ith element and $x_{\min}$ is a very small value (e.g. 0.001). x_{ij} is equal to 1 when the element is filled with material phase j or the constituent phases with larger stiffness/thermal conductivity and $x_{ij} = x_{\min}$ otherwise. As a result, the term $\sum_{i=1}^{M} x_{ij} V_i$ in Eq. (1) denotes the volume summation of the jth phase and stiffer phases ($j+1,\ldots,M$); the volume constraint in Eq. (1) means that the volume of the jth phase should be equal to the prescribed value, V^{j*}.

The physical property of the ith element is interpolated between two neighboring phases using a power-law scheme. For instance, the elemental elasticity matrix $\boldsymbol{D}$ can be interpolated as [22]:

$$\boldsymbol{D}(x_{ij}) = x_{ij}^p \boldsymbol{D}^j + (1 - x_{ij}^p) \boldsymbol{D}^{j+1} \tag{3}$$

in which the subscripts j and $j+1$ indicate the phase numbers and p is the penalty exponent which is usually equal to 3. Similarly the thermal conductivity of the ith element can be interpolated between two neighboring phases as:

$$\boldsymbol{\kappa} = x_{ij}^p \boldsymbol{\kappa}^j + (1 - x_{ij}^p) \boldsymbol{\kappa}^{j+1} \tag{4}$$

2.2. Homogenization theory and sensitivity analysis

For topology optimization of material's microstructures, it is necessary to calculate the macroscopic properties of the composite based on the distribution of constituent phases within its microstructure. If a heterogeneous composite possesses certain types of regularity at the microscale, its properties can be estimated by modeling the PBC with the help of the homogenization theory [24,25]. For example the homogenized elasticity matrix of materials with repeating (periodic) microstructures is expressed as: