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Design of composite structures with extremal elastic properties in the presence of technological constraints

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ABSTRACT

In this paper, composites made of periodically repeating micro structures are investigated. The study aims at identifying the optimal spatial distribution of constituents within a composite material to obtain the material of desired/improved functional properties. To find the relationship between micro- and macro-structural properties of the composite material, the method of homogenization is used. The problem of finding optimal microstructures of various materials, with the aim of obtaining maximum rigidity, i.e., maximum volume and shear modules for the base cell of a composite that contains the original installation of technological holes and/or inclusions was first investigated. For illustration and validation of the proposed approach, numerical examples are provided.

1. Introduction

It is well known that mechanical properties of composite materials can be improved by modifying the topology of the material microstructure. For instance, an approach based on the structural topology optimization can be employed to find the best space distribution of material phases constituting the composite microstructure. The main idea of designing a microstructure of a composite material having periodic patterns/cells is based on finding optimal distribution of periodic stress-strain fields already on a micro-scale, for a periodic elementary cell, called a base cell. A base cell can be studied with the help of the finite element method, and then a procedure of the topological optimization of this elementary, periodically repeated cell can be investigated instead of studying the whole composite structure. Usually, the method of homogenization is applied in order to average the complex micro structural behavior of an elastic medium to determine the macroscopic properties of a unit cell. The theory of homogenization has been recognized as a rigorous modeling methodology for characterizing the mechanical behavior of cellular materials and composites with periodic microstructures [1–3]. However, for complex microstructures of the elastic medium, analytical determination of the stress/strain fields is extremely difficult. Therefore, to find the most effective properties of the elastic medium, the homogenization procedure is employed by means of numerical approaches like the finite element method (FEM) [4,5].

The inverse problem is to design a new microstructure of the periodic unit cell so that the resulting material has desirable physical properties. The material design concept based on topology optimization and homogenization has been applied to design elastic [6–13] and thermo elastic [14,15] composite materials. A systematic and scientific means of microstructural design is formulated as an optimization problem for the parameters that represent the material properties and topology of the material microstructure.

Over the last two decades, various topology optimization algorithms and interpolation schemes, e.g. solid isotropic material with penalization (SIMP) [16–19], evolutionary structural optimization (ESO) [20], and level set technique [21,22] have been developed. These topology optimization techniques have been used extensively to solve design problems not only for macroscopic structures, but also for microstructures of materials/composites in recent years.

Some attempts have been also made to design new materials with extraordinary physical properties, e.g., extreme thermal conductivity [23] and maximum stiffness and thermal conductivity

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[24], designing a microstructure of functionally graded materials having their physical properties changing along with the gradient distribution of constituents [25].

In the above studies, the optimization was carried out for composites of one or two materials for a homogeneous base cell. In this work, maximization of static stiffness problem for a base cells composite materials, i.e. having maximum bulk modulus or shear modulus, has been considered. The problem of topological optimization for the base cell of the composite containing initially established technological holes and/or inclusions has been first solved. Topological optimization of reinforcing inclusions, embedded in a matrix with desired properties, is carried out only in the area of the base cell not connected with technological restrictions.

2. Definition of the effective elastic tensors of a base cell

The following assumptions are taken while carrying out the investigations: (i) an elastic composite is linear; (ii) the composite is microscopically (transversely) isotropic; (iii) there is a lack of initial stresses; (iv) the inclusions are homogenous, linear elastic, isotropic, and regularly packed; (v) the matrix material is homogenous, linear and isotropic.

Composites made from linear elastic materials are governed by linear equations of elasticity derived for a homogenized base cell.

In the elastic regime, the macroscopic behavior of a unit cell made from an anisotropic material can be characterized by the effective stress tensor $\bar{\sigma}_{ij}$ and the deformation tensor $\bar{\varepsilon}_{ij}$ of a homogenized medium, which are coupled by the so-called effective elasticity tensor C^{eff}_{ijkl} as follows:

$$\bar{\sigma}_{ij} = C^{eff}_{ijkl}\bar{\varepsilon}_{kl}, \tag{1}$$

where C^{eff}_{ijkl} depends on the filler volume fraction and properties of the base cell microstructure. In what follows, a local coordinate system (Y) is introduced with the use of the multiple scale method [1,2] in order to describe rapid changes in the material microstructure properties in the global coordinate system (X). In this method, the solution to the problem is searched in the form of a series of different powers of a small perturbation parameter ε with coefficients depending on variables x_i (called slow or macroscopic) and y_i (fast, microscopic variables). The mentioned series is substituted into the initial system of governing differential equations, and then the system is split into equations standing by the same powers of ε, which yield equations regarding the function u^i. Note that the function u^0 and the coefficients of equations with respect to u^0 are independent of fast variables. Here, a local coordinate y can be taken as a fast coordinate coupled with a slow coordinate x by the ratio $y = x/\varepsilon\,(\varepsilon << 1)$. Displacement of an arbitrary point of an elastic body can be approximated by a two-scale asymptotic expansion [1,2] of the form:

$$u^{\varepsilon}(x) = u^0(x,y) + \varepsilon u^1(x,y) + \varepsilon^2 u^2(x,y) + \ldots \tag{2}$$

Substitution of (2) into equilibrium equations yields the following effective tensor of elastic properties:

$$C^{eff}_{ijkl} = \frac{1}{|Y|}\int_Y \left(C_{ijkl} - C_{ijpq}\frac{\partial \chi^{kl}_p}{\partial y_q}\right)dy, \tag{3}$$

where $|Y|$ denotes the area of the base cell, χ^{kl}_p stands for $Y-$ periodic virtual displacements fields for the case of loading kl [1]. The index p ($p = 1, 2$) denotes the number of the coordinate of the virtual displacement (χ_1 and χ_2) while the index q ($q = 1, 2$) is the number of the local coordinate, i.e. either y_1 or y_2.

The following integral equation regarding the base cell with periodic boundary conditions holds:

$$\int_Y C_{ijpq}\frac{\partial \chi^{kl}_p}{\partial y_q}\frac{\partial v_i}{\partial y_j}dY = \int_Y C_{ijkl}\frac{\partial v_i}{\partial y_j}dY, \quad \forall \mathbf{v} \in Y, \tag{4}$$

where $\mathbf{v}$ stands for the (kinematically admissible) virtual displacement field.

The so far considered problem (4) is further solved for the base cell using the FEM. The corresponding compatibility conditions are formulated along the boundaries of different phases. In the plane stress state, there are three independent cases of load, i.e. $kl = 11,\ 22,\ 12$. Eq. (3) can be recast to the following form:

$$C^{eff}_{ijkl} = \frac{1}{|Y|}\int_Y \left(C_{ijkl} - C_{ijpq}\frac{\partial \chi^{kl}_p}{\partial y_q}\right)dY = \langle C_{ijkl}\rangle - \langle \sigma^{kl}_{ij}\rangle, \tag{5}$$

where $\langle C_{ijkl}\rangle$ denotes the average elastic tensor depending on the volume fraction of the used material. Its estimation is carried out according to the classical rule of material mixing, and $\langle \sigma^{kl}_{ij}\rangle$ denotes the average stress tensor associated with the base cell in the case of the load kl. Naturally, $\langle \sigma^{kl}_{ij}\rangle$ plays a role of the correction term reflecting the influence of the microstructure of the material elementary cell.

In a more understandable notation (5) may be written as [19,26]

$$C^{eff}_{ijkl} = \frac{1}{|Y|}\int_Y C_{pqrs}\left(\varepsilon^{0(ij)}_{pq} - \varepsilon^{*(ij)}_{pq}\right)\left(\varepsilon^{0(kl)}_{rs} - \varepsilon^{*(kl)}_{rs}\right)dy, \tag{6}$$

where $\varepsilon^{*(ij)}_{pq} = \frac{1}{2}\left(\frac{\partial \chi^{ij}_p}{\partial y_q} + \frac{\partial \chi^{ij}_q}{\partial y_p}\right)$ and $\varepsilon^{0(ij)}_{pq}$ are linearly independent unit test strains, which are applied to the base cell to determine the characteristic strain fields $\varepsilon^{*(ij)}_{pq}$. Three test strain fields are required for 2D problems. In 2D the test strain fields take the form of $\varepsilon^{0(11)}_{pq} = [1\,0\,0]$, $\varepsilon^{0(22)}_{pq} = [0\,1\,0]$ and $\varepsilon^{0(12)}_{pq} = [0\,0\,1]$ [7,27]. It is noted that due to symmetry, $\varepsilon^{0(12)}_{pq} = \varepsilon^{0(21)}_{pq}$ reducing the required test strains from four to three in 2D.

Note that, for an arbitrary microstructure, although C is isotropic, there is no reason for C^{eff} to be isotropic or orthotropic. However, many authors enforce the homogenized material to be isotropic or orthotropic. For microstructures having square symmetry (Fig. 1), the homogenized elastic tensor C^{eff} is orthotropic.

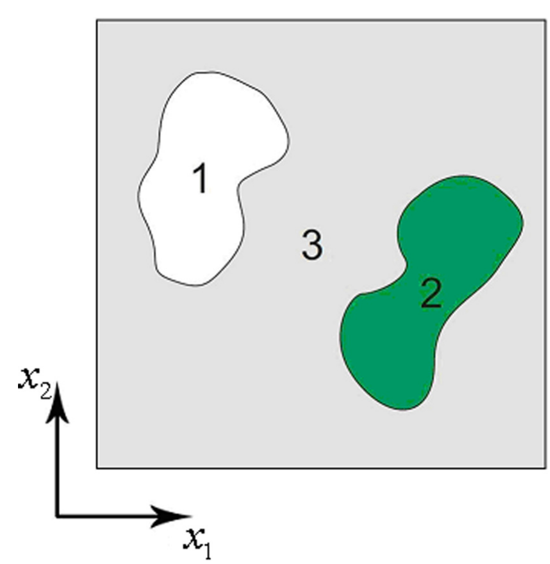

Fig. 1. Quarter base cell: 1 – technological hole; 2 – technological inclusion; 3 – domain of topological design.