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Research paper

Topological shape optimization of 3D micro-structured materials using energy-based homogenization method

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ABSTRACT

This paper proposes an effective method for the design of 3D micro-structured materials to attain extreme mechanical properties, which integrates the firstly developed 3D energy-based homogenization method (EBHM) with the parametric level set method (PLSM). In the 3D EBHM, a reasonable classification of nodes in periodic material microstructures is introduced to develop the 3D periodic boundary formulation consisting of 3D periodic boundary conditions, 3D boundary constraint equations and the reduced linearly elastic equilibrium equation. Then, the effective elasticity properties of material microstructures are evaluated by the average stress and strain theorems rather than the asymptotic theory. Meanwhile, the PLSM is applied to optimize microstructural shape and topology because of its positive characteristics, like the perfect demonstration of geometrical features and high optimization efficiency. Numerical examples are provided to demonstrate the advantages of the proposed design method. Results indicate that the optimized 3D material microstructures with expected effective properties are featured with smooth structural boundaries and clear interfaces.

1. Introduction

Micro-structured materials consist of a number of periodically arranged microstructures and possess some superior performance, such as the higher specific stiffness and strength, better fatigue strength and improved corrosion-resistance [1,2]. Currently, this kind of materials has gained extensive applications in various engineering fields. For example, the typical cellular honeycomb composites composed of an array of periodic unit cells (PUCs) have been employed in automobile and aerospace industries [3]. Although PUCs are fashioned with regular constituent materials, like metal and foam, many superior and extraordinary properties mentioned-above at the bulk scale can be presented. The main reason is that the macroscopic performance of cellular composites mainly depends on the configurations of PUCs rather than the constituent compositions [4,5]. Up to now, an increasing number of publications have reported on the modification of the geometrical sizes and shapes of microstructures to enhance their properties. However, these related existing methods are recognized to be experimental or intuitive [6].

Computational topology optimization has long been recognized as a powerful tool for the optimization of both structures and materials, which offers a systematic and scientific driven framework for design [7–10]. The basic idea is that materials are iteratively eliminated and redistributed within a given design domain to seek the best material distribution with the optimal performance under some prescribed constraints. This research field has undergone remarkable developments in recent years and various topology optimization methods have been developed, such as the homogenization method [11], solid isotropic material with penalization (SIMP) method [12,13], evolutionary structural optimization (ESO) method [14], and level set method (LSM) [15–17]. Meanwhile, since the homogenization theory [18] is developed to evaluate macroscopic effective properties based on the topologies of periodical material microstructures, it has become popular to combine the homogenization theory with topology optimization to formulate an inverse design procedure of PUCs for gaining the specific effective properties [19]. Many researchers have devoted considerable efforts to optimize or tailor material effective properties, so that micro-structured materials with various novel effective properties have been presented, such as the extreme mechanical properties [20–23], maximum stiffness and fluid permeability [24,25], exotic thermo-mechanical properties [26], negative Poisson's ratio (NPR) [27–30] and extreme thermal properties [31]. Micro-structured materials design has become one of the most promising applications of topology optimization [7,32].

In majority of the existing works for the optimization of PUCs, numerical homogenization method (NHM) works as the bridge between the design of materials and topology optimization to evaluate material effective properties. It is well-known that the asymptotic expansion

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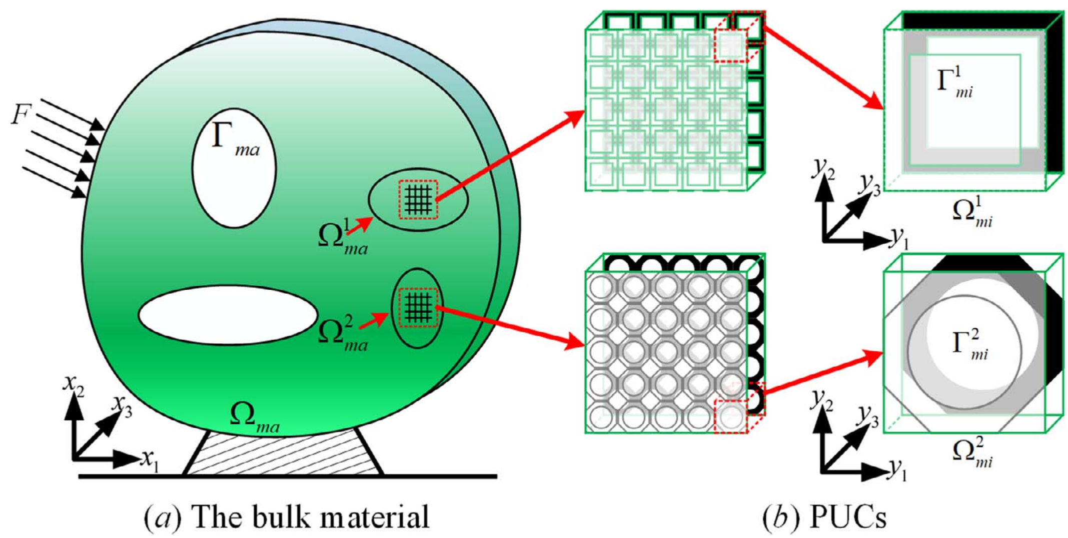

Fig. 1. The bulk material composed of two kinds of PUCs.

theory is the basic framework of the NHM, while its theoretical derivations and numerical implementations are complex [33,34]. For example, a fictitious body force is formulated under the imposing of the initial unit test strains on PUCs to solve the induced strain field in the finite element analysis [35]. Moreover, the NHM would be hard to be directly connected with topology optimization for materials design [28]. Hence, as an alternative way, the energy-based homogenization method (EBHM) with simple theoretical analysis and easy numerical implementations is proposed [28]. The key idea is that the average stress and strain theorems act as the theoretical basis to evaluate effective properties by reasonably imposing the initial unit test strains to construct the periodic boundary formulation. Until now, the EBHM gains great applications, such as combining with hybrid cellular automata [30], lattice structures [36], advanced structures and materials [37,38]. However, only the 2D periodic boundary formulation in the EBHM is developed to design 2D micro-structured materials with extreme effective properties. In the view of real-world engineering design problems, the design of 3D micro-structured materials is much more common and meaningful.

On the other side, the LSM is applied to optimize structures by evolving structural boundaries rather than material layouts in material distribution model, so that the optimized structures have smooth boundaries and are free of grayscales. Since the seminar work of Sethian and Wiegmann [15], the LSM has been quickly expanded to solve a broad range of optimization problems [39–41], including materials design [42,43]. However, due to directly solving the H-J PDE, some unfavorable numerical implementations with strict requirements are involved in the standard LSM [16,17] (e.g. Courant-Friedrichs-Lewy (CFL) condition, re-initialization and boundary velocity extension), which may hinder its further applications. In response to the numerical issues, many variants of the LSM are proposed [44–48]. One of them, termed as the parametric LSM (PLSM) [49,50], would be a powerful alternative LSM for handling topological shape optimization problems due to that the intrinsic desired features (e.g. the perfect demonstration of structural features) are kept while avoiding the difficulties of the LSM. The central idea is the interpolation of the level set function by a given set of the compactly supported radial basis functions (CSRBFs). Thus, the initial complicated PDE-driven shape topology optimization problem can be converted into a much easier "size" optimization problem. Moreover, many well-established optimization algorithms can be directly applied to evolve design variables, e.g. the optimality criteria (OC) method [12] and the method of moving asymptotes (MMA) [51]. Many optimization problems have been successfully solved by the PLSM, like the compliant mechanism [52], manufacturing constraints [53], robust optimization [54], multi-materials [55], and functional graded cellular composites [56].

In the present work, an effective design method for 3D micro-structured materials is proposed, where the 3D EBHM is developed to evaluate material effective properties and the PLSM is applied to evolve structural topologies. In the 3D EBHM, the 3D periodic boundary formulation is elaborated from three key factors: the imposing of the 3D periodic boundary conditions, the development of the 3D boundary constraint equations and the derivation of the reduced linearly elastic equilibrium equation. Firstly, the initial unit test strains are only imposed on the structural boundaries including the vertices, edges and surfaces of 3D microstructures to maintain the periodicity and continuity conditions in the bulk material. Then, a reasonable classification of nodes in a 3D PUC is defined to develop the boundary constraint equations, so that the periodic boundary conditions are illustrated in an explicit way to directly impose on the boundaries of PUCs. Finally, a direct solution scheme is employed to derive the reduced linearly elastic equilibrium equation for solving the displacement field in the finite element analysis. Due to the use of the PLSM, the optimized structures are free of the grayscales and zigzag interfaces, which are problematic in the engineering sense because the obtained optimal solutions are difficult to be interpreted as the manufacturable designs.

The remainder of this paper is organized as follows. A brief introduction about the homogenization theory is given in Section 2. Section 3 provides a detailed description of the 3D EBHM, including periodic boundary conditions, boundary constraint equations and the reduced linearly elastic equilibrium equation. In Section 4, the mathematical model of 3D micro-structured materials design is provided. Section 5 presents the detailed numerical implementations. Numerical examples are provided to illustrate the advantages of the proposed method in Section 6. Conclusions and further work are displayed in Section 7.

2. Homogenization theory

The homogenization theory is applied to evaluate material effective properties by directly analyzing the periodically distributed material unit cells, i.e., material microstructures. It includes two assumptions: (1) the dimensional sizes of PUCs are much smaller than that of the bulk material; and (2) PUCs are periodically distributed in the bulk material [33,34]. In the scope of linearly elastic material, the local coordinate system $\mathbf{y}$ is utilized to describe PUCs in the global coordinate system $\mathbf{x}$, shown in Fig. 1. It can be clearly seen that two kinds of PUCs are periodically arranged in different parts of the bulk material.