Computational Materials Science 87 (2014) 178–186

Contents lists available at ScienceDirect

Computational Materials Science

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

Topological shape optimization of microstructural metamaterials using a level set method

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ARTICLE INFO

Article history:
Received 1 December 2013
Received in revised form 3 February 2014
Accepted 6 February 2014
Available online 6 March 2014

Keywords:
Mechanical metamaterials
Artificial composite material
Microstructure
Level set method
Topological shape optimization

ABSTRACT

Metamaterials usually refer to artificial composite materials consisting of an array of periodically arranged microstructures, engineered to provide unusual material properties that may not be easily found in nature. This paper proposes a new topological shape optimization method for systematic computational design of a type of mechanical metamaterials with negative Poisson's ratios (auxetic materials), which integrates the numerical homogenization approach into a powerful parametric level set method (PLSM). The homogenization method is used to obtain the effective properties of the periodic microstructure, while the PLSM is applied to achieve shape evolutions and topological changes of the microstructure, until the desired material properties are achieved. The key concept of the PLSM is the interpolation of the implicit level set surface by using a given set of compactly supported radial basis functions (CSRBF), which are positioned at a number of given and fixed knots inside the design domain. Several typical numerical examples are used to demonstrate the favorable characteristics of the proposed method in the design of micro-structured metamaterials.

1. Introduction

Metamaterials [46,52] are artificial materials engineered to have unconventional effective properties that cannot be easily obtained in nature. They are usually characterized by assemblies of a number of periodic microstructures fashioned with conventional materials, such as metals or plastics. Thus the layout of the microstructure has a great impact on the properties of metamaterials. In general, metamaterials gain extraordinary properties from their microstructures rather than from their material composition. Due to the exotic properties, metamaterials are experiencing popularity in a number of new and emerging areas. Over the past two decades, several types of metamaterials have been developed for a diverse of applications in science and engineering, e.g. electromagnetic metamaterials [46,66,65,26,42], mechanical metamaterials [28,17,38] and acoustic metamaterials [11]. However, this paper is focused on the design of a family of elastic metamaterials with negative Poisson's ratios [28,38], which are also known as auxetic metamaterials (Evans and Alderson).

The Poisson's ratio of a solid is defined as the ratio of transverse contraction strain to longitudinal stretching strain under uniaxial tension. It is a fundamental metric to measure the performance of elastic materials and facilitates the contemporary understanding of the mechanical properties of modern materials [18]. Although the classic theory of elasticity allows the Poisson's ratio to be negative, most conventional materials in nature possess positive values. In contrast to materials with positive Poisson's ratios, negative Poisson's ratio materials exhibit counter-intuitive properties: expanding laterally when stretched and contracting laterally when compressed. Since the work (Lakes 25), the auxetic metamaterials have attracted increasing attention, due to their potential in a range of applications. However, only a limited number of natural materials [10,63] and artificial structures [43,17] have been reported to exhibit negative Poisson's ratios. Several intuitional and heuristic methods have been developed to generate auxetic metamaterials [62], but the systematic design approaches are still in demand for creating novel auxetic metamaterials.

In the past two decades, topology optimization has been expanding as a powerful computational design tool for a broad range of structures and materials [7,16,24,51]. Essentially, topology optimization is a numerical iterative process that distributes a given amount of material inside a fixed design domain to seek the best material layout, such that the objective function is optimized subject to a set of constraints. So far, there have been several methods developed for topology optimization of structures, e.g., the homogenization method [5,19,3], the evolutionary

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http://dx.doi.org/10.1016/j.commatsci.2014.02.006
0927-0256/

structural optimization method [58,25], the element density SIMP method [64,6], the nodal density SIMP approach [20,27,37], and the level set based method (LSM) [45,55,1]. Amongst a number of applications of topology optimization, one of the most promising applications may be the optimal design of micro-structured materials [47,48,50,21].

As aforementioned, since the layout of the microstructure plays an important role in determining the effective properties of the material, it is of great interest to apply topology optimization methods to achieve the optimal material layout of the periodic microstructure (unit cell). Several topology optimization methods can be used to design the unit cell of micro-structured materials in this field. For instance, the inverse homogenization method (IHM) [47] has been widely applied to achieve optimal topology of the periodic microstructure for the design of various metamaterials, such as the metamaterials with desired properties [47,29,14,66] or even extreme properties [48,22,50], and the metamaterials with multiphysics properties [21,26]. However, it can be seen that the above studies mainly based on the material density-distribution topology optimization methods [7]. The material density-based topology optimization methods have experienced considerable popularity due to their conceptual simplicity and numerical easiness [7]. However, there are several numerical instabilities to be carefully handled [49], they may result in optimized designs characterized with unfavorable numerical features [55,1,16,24], such as zigzag material interfaces and ambiguities of intermediate element densities. To facilitate the fabrication of the final design, additional post-processing schemes have to be employed to threshold element densities to enable a distinct, as well as a smooth interface.

The LSM [44,41] has recently emerged as a new method for shape and topology optimization of structures. After the pioneer's work of [45], several methods [1,2,55,56,60,61,12,15] have been developed for topological shape optimization within the context of standard LSM [40,44]. The standard level set methods have been applied to different design problems, including the design of acoustic [30] and photonic metamaterials [66,42], which may be less successful due to the intrinsic shortcomings of their design methods. One of the major concepts behind these LSMs is to represent the design boundary of a structure implicitly as the zero level set of a higher dimensional level set function (LSF). Then, the motion of the design boundary is mathematically described as a Hamilton–Jacobi partial differential equation (H–J PDE) [40], in which the normal velocity field to enable the evolution of the design boundary is often obtained using the shape derivative method [53,13]., one common characteristic of the above LSMs, categorized as conventional LSMs, is that they essentially track dynamic boundary by directly solving the H–J PDE using the finite difference method, e.g. up-wind schemes [55,1].

The LSMs can provide unique benefits in optimizing shape and topology of a structure, in particular, smooth boundary and distinct interface, shape fidelity and topological flexibility, integrated shape and topology optimization [55,1,32,16]. However, the conventional LSMs involve several unfavorable numerical features in topological shape optimization. For example, the global re-initializations are required to be periodically applied [55,1] to recover the signed-distance shape of the LSF, by avoiding the generation of a too steep or too flat LSF. Moreover, the CFL (Courant–Friedrichs–Lewy) condition must be satisfied to ensure the numerical stability in solving the H–J PDE [40,41]. Since the CFL condition states that each marching step size in space is no more than the smallest size of the grid, this will typically lead to a large number of iterations for a dense mesh. Furthermore, the final design will largely depend on the initial guess, due to no mechanism being included to create new holes inside the domain [9]. It is noted that [32,16,39] these issues have limited the further application of LSMs to more advanced topological shape optimization problems.

More recently, several alternative LSMs (e.g., [4,23,31–36]) have been developed for topological shape optimization of structures, to avoid the above numerical issues in the conventional LSMs. One of the common features in these LSMs is to optimize the shape and topology of structures, without directly solving the H–J PDE using up-wind schemes. In particular, [32,31] have proposed a parametric level set method (PLSM) for topological shape optimization of continuum structures. In this method, the compactly supported radial basis function (CS-RBF) [8,57] was utilized to achieve the interpolation of the implicit LSF, and then the design boundary was advanced by iteratively updating a set of unknown expansion coefficients of the interpolant. The PLSM has shown its ability as a powerful topological shape optimization method for structures [32,31], which can remain the favorable while avoid unfavorable numerical issues of the conventional LSMs. Particularly, many well-established gradient-based optimization algorithms, including the optimality criteria (OC) [4,32] and mathematical programming methods [23,31] an be directly applied to the LSMs.

This paper will develop a new topological shape optimization method for computational design of mechanical metamaterials, which systematically integrate the numerical homogenization method that is used to predict the material effective properties, with the PLSM that is employed to optimize the shape and topology of the unit cell. The proposed method shows unique merits, especially suits the topological shape design of micro-structured artificial composites. In particular, the proposed method naturally bridges the level set equation with many more effective and efficient optimization algorithms, compared to the original PDE-driven topological shape optimization using the finite difference method (FDM). Furthermore, the proposed method is general, because it can be applied to design other elastic metamaterials, as well as photonic and phononic (seismic, acoustic) metamaterials. This paper is the first time to extend the PLSM to the design of metamaterials. Several numerical examples will be presented to demonstrate the effectiveness of the proposed method in the optimal design of engineered metamaterials.

2. Parametric level set method

2.1. Level set-based boundary representation

As mentioned above, in the level set-based structural optimization methods, the first element is to implicitly represent the design boundary of a structure by the zero level set of a higher dimensional LSF with Lipschitz continuity [40]. For instance, Fig. 1 shows the representation of a two-dimensional boundary with a three-dimensional level set surface, where ϕ is used to denote different parts of the reference domain, as follows:

$$\begin{cases} \varphi(\mathbf{x}) > 0 & \forall \mathbf{x} \in \Omega \setminus \Gamma & \text{(solid region)} \\ \varphi(\mathbf{x}) = 0 & \forall \mathbf{x} \in \Gamma & \text{(design boundary)} \\ \varphi(\mathbf{x}) < 0 & \forall \mathbf{x} \in D \setminus (\Omega \cup \Gamma) & \text{(void region)} \end{cases} \quad (1)$$

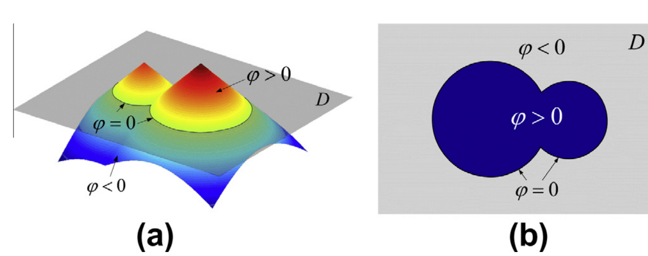

Fig. 1. (a) Three-dimensional LSF; and (b) design domain with the zero level set.