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Designing orthotropic materials for negative or zero compressibility

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ABSTRACT

There has been considerable interest in materials exhibiting negative or zero compressibility. Such materials are desirable for various applications. A number of models or mechanisms have been proposed to characterize the unusual phenomena of negative linear compressibility (NLC) and negative area compressibility (NAC) in natural or synthetic systems. In this paper we propose a general design technique for finding metamaterials with negative or zero compressibility by using a topology optimization approach. Based on the bi-directional evolutionary structural optimization (BESO) method, we establish a systematic computational procedure and present a series of designs of orthotropic materials with various magnitudes of negative compressibility, or with zero compressibility, in one or two directions. A physical prototype of one of such metamaterials is fabricated using a 3D printer and tested in the laboratory under either unidirectional loading or triaxial compression. The experimental results compare well with the numerical predictions. This research has demonstrated the feasibility of designing and fabricating metamaterials with negative or zero compressibility and paved the way towards their practical applications.

1. Introduction

Compressibility is a measure of the relative volume change of a solid or fluid as a response to a pressure change. Usually a material contracts in all directions when the pressure increases. However there are some exceptional materials which expand under hydrostatic pressure in one or two directions. Such phenomena are known as negative linear compressibility (NLC) and negative area compressibility (NAC), respectively. In recent years, there has been increasing interest in the negative compressibility behavior, mostly due to its many potential applications such as sensitive pressure sensors, pressure driven actuator and optical telecommunication cables. At the molecular or nanostructural level, a few materials displaying NLC have been found, e.g. $Ag_3[Co(CN)_6]$ (Goodwin et al., 2008), methanol monohydrate (Fortes et al., 2011; Grima et al., 2011b), zinc dicyanoaurate (Li et al., 2012). At the micro and macro levels, Baughman et al. (1998) have proposed a wine-rack mechanism to explain the NLC effect. Weng et al. (2008) have presented a list of crystals that exhibited NLC. Barnes et al. (2012) have proposed tetragonal beam structures which display NLC effect. One mechanical property which may accompany NLC or NAC is the negative Poisson's ratio (i.e. auxetic). This has been investigated based on a model of 2D hexagonal honeycomb which is similar to certain types of open cell foams (Nkansah and Hutchinson, 1994) (Grima et al., 2011a). The 3D equivalence of the honeycomb is an elongated hexagonal dodecahedron system. Grima et al. (2012) have presented a detailed analysis of the system to assess the auxetic and NLC/NAC effect.

An immediate application of NLC/NAC materials is the optical component in interferometric pressure sensors due to the higher sensitivity achieved by a combination of large volume compressibility with negative linear compressibility (Cairns et al., 2013). With further understanding the mechanisms of negative compressibility, NLC/NAC materials also have potential to be used as efficient biological structures, nanofluidic actuators or as compensators for undesirable moisture-induced swelling of concrete/clay-based engineering materials (Cairns et al., 2013).

It is noted that all the above known NLC and NAC materials have a pre-determined topology. If the topology of the material microstructure is allowed to be changed or "designed", it opens up many possibilities for finding new materials with NLC/NAC effect. There has been extensive work on material design using topology optimization, covering various properties such as stiffness,

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Nomenclature

$\mathbf{E}$	the elastic matrix of the base material
$\mathbf{E}^H$	the homogenized (effective) elasticity matrix of cellular material
E_{ij}^H	the effective elastic constants
$\mathbf{C}^H$	the homogenized compliance matrix (the inverse of $\mathbf{E}^H$)
C_{ij}	the effective compliance constants
NE	the number of elements
$\boldsymbol{\varepsilon}_i^0$	the ith unit strain field
Y_e	the volume of the given domain
$\boldsymbol{\varepsilon}_i$	the induced strain field
β_{Li}	the linear compressibility in axis i (i = 1, 2, 3)
β_{Aij}	the area compressibility in the ij plane
β_v	the volume compressibility
p	a stress factor or a penalty parameter
p^{upper}	the upper bound of p
V	the prescribed total volume
V_e	the volume of element e
V^k	the total volume at iterations k
x_e	the design variable, with $x_e = x_{\min}$ for void and x_e = 1 for solid
λ	Lagrangian multiplier
E_{b1}	the Young's modulus of the base materials 1
E_{b2}	the Young's modulus of the base materials 2
q	a penalty factor, with typical values being equal to or greater than 3
$r_{\min}$	the minimum filter radius
α_e	the sensitivity number of element e
$\tilde{\alpha}_e$	the weighted average sensitivity number of element e
NR	the total numbers of elements removed
NA	the total numbers of elements added
NE_{thre}	the number of elements above the threshold
$AR_{\max}$	the maximum allowable number of elements added in one iteration
$R_{\max}$	the maximum allowable ratio of elements added or removed in one iteration
$\boldsymbol{\varepsilon}$	the induced strain field
f_L	the Lagrangian function
$\frac{1}{E^*}$	the compliance constraint
f_{con}	the stiffness constraint
E_i	Young's modulus in direction i
v_{ij}	Poisson's ratios in the ij plane
$\boldsymbol{\sigma}$	the stress vector
Π	the general objective function
E_0	Young's modulus of TangoPlus material
μ_0	Poisson's ratio of TangoPlus material
E_m	Young's modulus of the cover material used in triaxial tests
μ_m	Poisson's ratio of cover material used in triaxial tests

acoustics, conductivity and permeability (Bendsøe and Sigmund, 2003). A recent study has used topology optimization for designing electromagnetic materials with negative permeability (Zhou et al., 2011). However, to the authors' best knowledge, there has been no work reported on systematic design of NLC/NAC materials using topology optimization. In this study, we shall develop a general technique for designing materials with negative or zero compressibility using topology optimization.

The optimization method used here is based on the bi-directional evolutionary structural optimization (BESO). The basic idea of BESO is that by gradually removing inefficient material from a ground structure and redistributing the material to the most critical locations, the structure evolves towards an optimum. For a 3D continuum material the ground structure is a unit cubic cell and the material properties (e.g. elasticity matrix) is determined using the homogenization theory (Hassani and Hinton, 1998). The extensive work on BESO has been presented in various publications (Huang and Xie, 2010; Querin et al., 1998; Yang et al., 1999). BESO has also been successfully applied to a wide range of material design problems, e.g. maximum bulk or shear modulus (Huang et al., 2011), tailored stiffness orthotropy (Yang et al., 2013), functionally graded materials (Radman et al., 2013) and multi-scale design of composite materials and structures (Zuo et al., 2013). These materials can be constructed as arrays of microstructures and then fabricated using advanced manufacturing technologies such as additive manufacturing (Challis et al., 2010).

Here we apply the BESO method to the design of materials of four types, namely, NLC, NAC, zero linear compressibility (ZLC) and zero area compressibility (ZAC). The mathematical formulation, optimization procedure and various examples are presented. A physical prototype of one of designed materials is fabricated using a 3D printer and tested in the laboratory under both unidirectional loading and triaxial compression. The experimental results are compared with the numerical predictions.

2. Determining linear, area and volume compressibilities of a material by homogenization

A cellular material consisting of a base material and voids is often modeled as a microstructure of a periodic base cell (PBC) using finite element (FE) analysis. According to the homogenization theory (Hassani and Hinton, 1998), the effective elastic constants can be expressed as

$$E_{ij}^H = \sum_{e=1}^{NE}\left(\frac{1}{Y_e}\int_{Y_e}(\boldsymbol{\varepsilon}_i^{0^T} - \boldsymbol{\varepsilon}_i^T)\mathbf{E}(\boldsymbol{\varepsilon}_j^0 - \boldsymbol{\varepsilon}_j)dY_e\right) \quad (i,j = 1 \text{ to } 6 \text{ for 3D}) \tag{1}$$

where $\mathbf{E}$ is the elastic matrix of the base material, NE is the number of elements, $\boldsymbol{\varepsilon}_i^0$ is the ith unit strain field, Y_e is the volume of the given domain and $\boldsymbol{\varepsilon}_i$ is the corresponding induced strain field. The implementation of the homogenization has become a standard procedure, as detailed in many publications, e.g. Hassani and Hinton (1998). For 3D materials, it involves applying six cases of periodic boundary conditions and unit strain fields. Then the 6×6 E_{ij}^H make up the elasticity matrix $\mathbf{E}^H$. The homogenized compliance matrix $\mathbf{C}^H$ is the inverse of $\mathbf{E}^H$, i.e.

$$\mathbf{C}^H = [C_{ij}] = \mathbf{E}^{H^{-1}} \tag{2}$$

As the materials studied here is orthotropic, there is no axial-shear coupling and thus the 3×3 sub-matrix of the axial components can be extracted as below

$$\mathbf{C}_A^H = [C_{ij}^A] = \begin{bmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{bmatrix} = \mathbf{E}_A^{H^{-1}} \tag{3}$$

The linear compressibility in direction i is defined as the relative change of strain i with respect to the change of the hydrostatic pressure dp (Grima et al., 2012), that is,