

Journal of the Mechanics and Physics of Solids

journal homepage: <www.elsevier.com/locate/jmps>

Design of materials with prescribed nonlinear properties

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article info

Article history: Received 5 September 2013 Received in revised form 17 March 2014 Accepted 5 May 2014 Available online 14 May 2014

Keywords: Material design Finite deformation Nonlinear properties Optimization

ABSTRACT

We systematically design materials using topology optimization to achieve prescribed nonlinear properties under finite deformation. Instead of a formal homogenization procedure, a numerical experiment is proposed to evaluate the material performance in longitudinal and transverse tensile tests under finite deformation, i.e. stress–strain relations and Poisson's ratio. By minimizing errors between actual and prescribed properties, materials are tailored to achieve the target. Both two dimensional (2D) truss-based and continuum materials are designed with various prescribed nonlinear properties. The numerical examples illustrate optimized materials with rubber-like behavior and also optimized materials with extreme strain-independent Poisson's ratio for axial strain intervals of $\varepsilon_i \in [0.00, 0.30]$.

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1. Introduction

Novel materials with special properties are highly attractive for modern technology. This comprises materials with exotic mechanical properties ([Lakes, 1987](#page--1-0); [Evans, 1991;](#page--1-0) [Safari, 1994\)](#page--1-0) and materials with enhanced electric and magnetic properties ([Scarpa and Smith, 2004](#page--1-0); [Shvets and Urzhumov, 2005](#page--1-0)). Materials with negative Poisson's ratio (NPR), known as auxetic materials, are one type of materials with unusual mechanical properties. In contrast to conventional materials, such materials will expand instead of shrinking when stretched. NPR materials have been demonstrated to exhibit enhanced shear resistance, indentation resistance [\(Alderson et al., 1994,](#page--1-0) [2000](#page--1-0)) and fracture toughness [\(Choi and Lakes, 1996](#page--1-0)). Moreover, NPR materials have been shown to possess extraordinary damping properties [\(Chen and Lakes, 1996\)](#page--1-0), acoustic properties ([Chekkal et al., 2010](#page--1-0)) and dynamic crushing performance ([Scarpa et al., 2002](#page--1-0)). Hence, NPR materials find potential applications in many fields [\(Lakes, 1993](#page--1-0); [Liu, 2006](#page--1-0)).

Besides natural NPR materials found in some rocks and minerals, a wide variety of auxetic materials have been created and fabricated using different deformation mechanisms ([Lakes, 1991](#page--1-0)), including polymeric and metallic foams [\(Lakes, 1987](#page--1-0)), microporous polymers ([Evans, 1991;](#page--1-0) [Alderson and Evans, 1992](#page--1-0)), carbon fiber laminates ([Evans et al., 2004](#page--1-0)) and honeycomb structures [\(Prall and Lakes, 1997](#page--1-0); [Lakes and Witt, 2002\)](#page--1-0). Under finite deformation, material properties are generally dependent on the deformation and show severe nonlinear behavior [\(Prall and Lakes, 1997](#page--1-0); [Smith et al., 1999](#page--1-0); [Scarpa and](#page--1-0) [Smith, 2004](#page--1-0)). Therefore, the optimized properties, such as NPR, based on small deformation theory may degrade or even reverse under finite deformation. Recently, periodic nonlinear affine unimode metamaterials have been constructed from

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rigid bars and pivots to achieve fixed Poisson's ratio over a large strain range ([Milton, 2013](#page--1-0)). In this study, we will investigate material design under finite deformation using topology optimization.

Over the last two decades, topology optimization methods have been demonstrated to be an attractive design approach in many fields covering mechanical and structural engineering, fluid dynamics, optical engineering, and more ([Bendsøe and](#page--1-0) [Kikuchi, 1988](#page--1-0); [Bendsøe and Sigmund, 2003\)](#page--1-0). Topology optimization has also shown its applicability to create novel materials with enhanced properties. In this way, material properties are tailored through a redistribution of the material layout in the microstructure. Examples include NPR materials ([Sigmund, 1994](#page--1-0), [1995](#page--1-0); [Larsen et al., 1997](#page--1-0); [Schwerdtfeger et al., 2012](#page--1-0); [Andreassen et al., 2014](#page--1-0)), materials with negative thermal expansion coefficient ([Sigmund and Torquato, 1997](#page--1-0)), novel piezoelectric properties [\(Silva et al., 1998](#page--1-0); [Sigmund et al., 1998\)](#page--1-0), enhanced dissipation ([Yi et al., 2000](#page--1-0); [Andreasen et al.,](#page--1-0) [2014](#page--1-0)), photonic and phononic bandgap materials ([Cox and Dobson, 1999](#page--1-0); [Sigmund and Jensen, 2003\)](#page--1-0) and metamaterials with negative permeability ([Diaz and Sigmund, 2010\)](#page--1-0). Moreover, in order to ensure manufacturability and control of minimum feature sizes of the topology optimized designs, different techniques have been developed ([Haber et al., 1996](#page--1-0); [Bourdin, 2001;](#page--1-0) [Bruns and Tortorelli, 2001;](#page--1-0) [Sigmund, 2007](#page--1-0), [2009](#page--1-0); [Wang et al., 2011\)](#page--1-0).

So far most examples of topological material design have been performed using linear finite element analysis valid for small displacements and linear elasticity. In this case the effective material properties can be computed by a standard homogenization approach for unit cells of periodic microstructures, see e.g. the review in [Hassani and Hinton \(1998a](#page--1-0)–c). A homogenization theory for the effective properties of nonlinear composite materials has been presented by [Talbot and](#page--1-0) [Willis \(1985\)](#page--1-0) and [Ponte Castañeda \(1991\)](#page--1-0). However, determining the homogenized properties of nonlinear materials at finite deformation is still an active research area. Important contributions in this field have been made by [Hill \(1972\)](#page--1-0), [Ponte](#page--1-0) [Castañeda and Zaidman \(1996\)](#page--1-0), [Miehe \(2003\),](#page--1-0) [Yvonnet and He \(2010\)](#page--1-0), [Lamari et al. \(2010\),](#page--1-0) and [Clement et al. \(2012\)](#page--1-0). Due to the complexity of the homogenization procedure under finite deformation, topology optimization methods have only recently been extended to tailor materials for prescribed nonlinear properties. In [Nakshatrala et al. \(2013\)](#page--1-0) the effective material properties are evaluated under finite deformation using a numerical homogenization procedure and incorporated into multiscale topology optimization that allows for locally varying microstructures.

The present study is closely related to the work of [Nakshatrala et al. \(2013\).](#page--1-0) However, we will focus on design of materials with prescribed stress–strain curves and Poisson's ratio under finite deformation. We restrict ourselves to material design based on numerical tensile experiments where the material is uniformly stretched, which allows us to circumvent the computationally intensive nonlinear homogenization. The geometrically nonlinear behavior of the periodic microstructure is simulated using a total Lagrangian finite element formulation, and solved by a Newton–Raphson algorithm. Two optimization problems of prescribed stress–strain curves and Poisson's ratio are formulated to minimize the errors between actual and prescribed properties for a target axial strain range. Two dimensional truss-based and continuum materials are designed using the proposed optimization formulation.

As an additional challenge, previous studies on structural topology optimization under finite deformation for stiffness optimization and design of compliant mechanisms ([Buhl et al., 2000](#page--1-0); [Pedersen et al., 2001](#page--1-0); [Bruns and Tortorelli, 2003](#page--1-0); [Yoon](#page--1-0) [and Kim, 2005;](#page--1-0) [Klarbring and Str](#page--1-0)o[mberg, 2013\)](#page--1-0), have shown that excessive deformation observed in low density elements may lead to numerical instability of the Newton–Raphson solution procedure. Different computational approaches have been introduced to circumvent the numerical instability ([Buhl et al., 2000;](#page--1-0) [Bruns and Tortorelli, 2003](#page--1-0); [Yoon and Kim, 2005](#page--1-0)). More recently, hyperelastic material models have been employed in structural topology optimization [\(Klarbring and](#page--1-0) [Stromberg, 2013](#page--1-0)) to remedy the problem. This approach works well for problems that are dominated by tensile forces and we have adapted this approach for our continuum examples where this is the case. For problems involving significant compression of void regions we have recently proposed a new interpolation scheme based on a linear modeling of the void regions [\(Wang et al., 2014\)](#page--1-0).

The paper is organized as follows. In Section 2, we introduce the physical model to characterize the material properties in a tensile test under finite deformation and state the corresponding finite element formulation. In [Section 3](#page--1-0), we formulate the optimization problems for designing materials with prescribed stress–strain curves and with prescribed Poisson's ratio for both truss-based and continuum materials. [Section 4](#page--1-0) is dedicated to presenting optimized material layouts for prescribed nonlinear properties as well as the corresponding performances. The paper ends with the conclusions in [Section 5.](#page--1-0)

2. Characterization of material behavior in a tensile test

In a periodic material, effective material properties can be characterized using a unit cell as illustrated in [Fig. 1\(](#page--1-0)a). Homogenization methods can be used to calculate the effective material properties in the small deformation regime. However, when the material undergoes finite deformation, the material properties will be strongly dependent on the deformation and the effective material properties have to be calculated for each deformation state [\(Yvonnet et al., 2009](#page--1-0)). In order to simplify the problem, this paper focuses on tensile deformation tests.

In a tensile test, materials are uniformly stretched either longitudinally or transversely. The material behavior can be characterized using the unit cell subjected to boundary displacements as shown in [Fig. 1\(](#page--1-0)b) and stated in Eq. [\(1\).](#page--1-0) The unit cell is fixed at the lower left corner. For each node pair on the left and right boundaries, periodic boundary conditions are employed in the transverse displacements, given as $v_1 = v_{01}$, and a constant displacement difference, u, is assumed longitudinally as $u_1 - u_{01} = u$. For each node pair on the lower and upper boundaries, periodic boundary conditions are

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