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Topology optimization of structures with length-scale effects using elasticity with microstructure theory

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This paper presents topology optimization of structures with inclusion of microstructural effects. To this end, Mindlin's elasticity with microstructure theory is used for investigating the scale effects. For implementation of finite element based topology optimization, a separate interpolation scheme for the displacement and micro-deformation field is adopted based on 8-node quadrilateral element. Numerical results show that although the continuum is associated with material length-scales, the minimal topological length-scale cannot be controlled without using a regularization technique. Results demonstrate that the length-scale of the microstructure may have a significant influence on the optimal topologies.

1. Introduction

Topology optimization is a process of finding the best layout of a given amount of material within a design domain for achieving desirable performance. Unlike the traditional size and shape optimization which usually takes member cross-sectional areas, thicknesses or geometric features as design variables for a predefined structural configuration, topology optimization is more flexible and allows designers to create more efficient and novel structural designs [1,2]. From the mechanics point of view, most of the studies for structural topology optimization in the past have been carried out with classical elastic theories which are applicable at macroscale where the microscale effects are negligible and can be ignored. It is well understood that every material relevant to engineering has its own microstructure, e.g. polymers are composed of molecular chains, polycrystalline materials consist of crystallites and granular materials have a grain structure. Generally if a structure under consideration has much larger physical dimensions than its characteristic microstructural dimensions, the classical elastic continuum mechanics theory suffices, wherein only the macrostructure behavior is considered and microstructure effects are ignored [3]. However, if dimensions of a structure are comparable to its corresponding material microstructure dimension, e.g. micro-devices in microelectromechanical systems (MEMS), the microstructural behavior may influence the final design. Experiments have reported that microstructural effects become increasing dominant if size of the structure is comparable to the characteristic microstructural dimensions, which is also known as the length-scale effect [4,5]. Since the classical continuum mechanics theories lack microstructural length-scale information, they are unable to reproduce the observed behavior from the experiments, and therefore, not able to capture the correct response in cases where length-scale effects are prominent. In such cases, the final topology designs using linear elastic theories can be inaccurate and even completely incorrect.

In order to model the microstructure length-scale effects, Cosserat brothers [6] first proposed the linear elastic constitutive model based on a continuum with microstructure in the early 20th century. In this theory every material particle is considered as a perfectly rigid volume and there are 3 displacement and 3 micro-rotation components during the deformation so that there are 6 degrees of freedom in total for each material particle. Based on Cosserat's theory, Toupin [7] proposed the linear couple-stress theory by eliminating the symmetric part of the strain gradient, and the high-order gradient terms were introduced. In 1960s, Mindlin [8] formulated a very general theory of elasticity with microstructure based on Cosserat and Toupin's work. In Mindlin's theory, there are 3 macroscale and 9 microscale deformations for each material particle. In this theory, kinematics and kinetics of the system are considered at both macroscale and microscale. In spite of its generality to describe the length-scale effects, Mindlin's theory is complex with too many material parameters. However, Mindlin's theory can also be simplified by making

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additional assumptions to construct gradient elasticity theories that require only one length-scale parameter, see for instance Ref. [3,8–11].

In contrast to the abundant research on topology designs based on linear elastic continua, little attention has been paid to topology design of structures wherein microstructure effects are critical. In this study, topology optimization is investigated for structures wherein the microstructural effects are significant. To this end, Mindlin's elasticity with microstructures theory [8] is used to incorporate material length-scale effects. Distinct finite element interpolations for macro and micro displacement fields are used in this study based on the interpolation scheme recently proposed by Zervos [9]. The microstructural length-scale effects on the optimal topology designs is studied through parametric studies wherein material parameters are systematically categorized at different length-scales. Finally, the influence of different length-scale parameters on the final optimal topologies and objective values are systematically presented and discussed.

The outline of this paper is as follows: Section 2 gives a brief review of Mindlin's [8] theory of elasticity with microstructures and Section 3 presents the finite element discretization scheme for implementing this theory. In Section 4 the convergence study of the element used in topology optimization is carried out and Section 5 presents the implementation of topology optimization problems. The numerical results are presented in Section 6, and finally the important conclusions and remarks are given in Section 7.

2. Elasticity with microstructure

In this section the basic theoretical framework for linear elasticity with microstructure is briefly presented; further details can be found in the original paper by Mindlin [8]. Tensor index notation is used throughout together with the usual summation convention. The kinematics and the kinetics are considered at both macro and micro levels.

2.1. Kinematics

Consider a material volume V which is bounded by surface S. In a Cartesian coordinate system with fixed origin, the position vector of each material particle is defined by vector x_i and the corresponding macro displacement field is expressed by $u_j(x_i)$ $(i = 1,\ 2,\ 3)$. Then the macro-deformation gradient ξ_{ij} is defined as follows:

$$\xi_{ij} = \frac{\partial u_j}{\partial x_i} \equiv u_{j,i} \tag{1}$$

The usual strain field ε_{ij}, termed as macroscopic strain, is defined as the symmetric part of macro-deformation gradient as follows:

$$\varepsilon_{ij} = \frac{1}{2}\left(u_{j,i} + u_{i,j}\right) \tag{2}$$

In elasticity with microstructure theory, a micro-volume V' is embedded at each material particle. The position of particles within this micro-volume is defined with respect to a new axes system that is parallel to the macroscopic coordinates x_i with origin moving with the material particle. In this micro-volume, the position of a particle is described by a vector x'_i and the corresponding micro-displacement field is defined by $u'_j(x_r, x'_k)$. For describing the micro-displacement field, in the simplest case, the following linear relationship between the position vector and the micro displacement field is assumed:

$$u'_j(x_r, x'_k) \stackrel{\text{def}}{=} x'_k \psi_{kj}(x_r) \tag{3}$$

where $\psi_{ij}(x_r)$ is the displacement gradient of the micro-medium defined as:

$$\psi_{ij}(x_r) = \frac{\partial u'_j}{\partial x'_i} \tag{4}$$

The symmetric part of ψ_{ij} is defined as the micro-strain tensor:

$$\varepsilon'_{ij} \stackrel{\text{def}}{=} \frac{1}{2}\left(\psi_{ij} + \psi_{ji}\right) \tag{5}$$

Finally, the relative deformation gradient γ_{ij} and micro-deformation gradient κ_{ijk} are defined as follows:

$$\gamma_{ij} = \xi_{ij} - \psi_{ij} \tag{6}$$

$$\kappa_{ijk} = \frac{\partial \psi_{jk}}{\partial x_i} \equiv \partial_i \psi_{jk} \tag{7}$$

The concept of relative deformation, which is the bridge between micro and macro scale deformation, is illustrated in Fig. 1. Consider a 2-D rectangular macro element $(\Delta x_1 \times \Delta x_2)$ which is composed of microstructures $(\Delta x'_1 \times \Delta x'_2)$ as shown in Fig. 1(a) and (b); note that both macrostructure and microstructure have their own coordinate systems, i.e. x_i and x'_i respectively. Now when the macro element domain is under relative axial stress τ_{22}, the relative deformation gradient is $\gamma_{22} = u_{2,2} - \psi_{22}$ (Fig. 1(a)). Similarly, when the macro element is under relative shear stress τ_{12}, there will be a relative deformation gradient $\gamma_{12} = u_{1,2} - \psi_{12}$ between macro-deformation gradient $u_{2,1}$ and micro-deformation gradient ψ_{12} (Fig. 1(b)).

2.2. Kinetics and potential energy

Potential energy density (W) per unit macro volume is assumed to be a homogeneous and quadratic function of forty-two variables $\varepsilon_{ij}, \gamma_{ij}$ and κ_{ijk}, i.e. $W = W\left(\varepsilon_{ij}, \gamma_{ij}, \kappa_{ijk}\right)$. By taking derivatives of the potential energy density, the three stress-like constitutive quantities are obtained as follows [8]:

$$\begin{aligned} \sigma_{ij} &= \frac{\partial W}{\partial \varepsilon_{ij}} \\ \tau_{ij} &= \frac{\partial W}{\partial \gamma_{ij}} \\ \mu_{ijk} &= \frac{\partial W}{\partial \kappa_{ijk}} \end{aligned} \tag{8}$$

where σ_{ij} can be interpreted as the usual Cauchy stress tensor that is conjugate to macro-strain $\varepsilon_{ij}, \tau_{ij}$ is the relative stress tensor that is conjugate to relative-strain γ_{ij}, and μ_{ijk} is the double stress tensor that is conjugate to micro-deformation gradient κ_{ijk}. Finally, four types of external forces are considered: body force (b_i) and surface tractions $(\tilde{t}_i)$ that are work conjugate to the displacement field, and body double force (ϕ_{ij}) and surface double force $(\tilde{T}_{ij})$ that are work conjugate to the micro-deformation gradient. By ignoring the inertia forces and considering the first variation of the total potential energy to be zero for arbitrary variations in the displacement and the micro-deformation gradient fields, the following equations of motion in V are obtained [8]:

$$\begin{aligned} \partial_i\left(\sigma_{ij} + \tau_{ij}\right) + b_j &= 0 \\ \partial_i \mu_{ijk} + \tau_{jk} + \phi_{jk} &= 0 \end{aligned} \tag{9}$$

together with the corresponding boundary conditions on S:

$$\begin{aligned} n_i\left(\sigma_{ij} + \tau_{ij}\right) &= \tilde{t}_j \\ n_i \mu_{ijk} &= \tilde{T}_{jk} \end{aligned} \tag{10}$$