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On optimal zeroth-order bounds of linear elastic properties of multiphase materials and application in materials design

Mauricio Lobos*, Thomas Böhlke

Chair for Continuum Mechanics, Institute of Engineering Mechanics, Karlsruhe Institute of Technology (KIT), Kaiserstr. 10, 76131 Karlsruhe, Germany

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ABSTRACT

Zeroth-order bounds of elastic properties have been discussed by Kröner (1977) and by Nadeau and Ferrari (2001). These bounds enclose the effective linear elastic properties of multiphase materials constituted of materials with arbitrary symmetry and of an arbitrary number of phases by using solely the material constants of the single materials. Nadeau and Ferrari showed that these bounds are isotropic tensors and presented an algorithm for the determination of the upper and the lower zeroth-order bound. It is shown in this paper that a problem arises for the lower bound, since the algorithm presented in Nadeau and Ferrari (2001), results in a negative compression modulus and/or shear modulus although the considered stiffness is positive definite. A simple analytic example for this undesirable property is given, together with a short *Mathematica*® code of the algorithm. In the present work, the definition of the lower bound by Nadeau and Ferrari is modified, thereby assuring its positive definiteness. The *Mathematica*® code of the corrected algorithm is also given. Furthermore, new bounds for non-diagonal components are derived, which give information of, in principle, accessible values for non-diagonal stiffness components using the zeroth-order bounds of the present work. The practical application of zeroth-order bounds for local and online material data bases of stiffness tensors is presented, in order to accelerate purposes in materials design through efficient materials screening.

1. Introduction

Multiphase materials (e.g., fiber reinforced polymers, particle reinforced materials, metal matrix composites, etc.) offer a rich pool of design options, see, e.g., Torquato (2002), Kainer (2006), Ashby (2010) and Adams et al. (2013). In the field of materials research, the development of accurate models predicting the anisotropic multi-physical material response of multiphase materials has been driven on in many ways. Novel experimental techniques allow a more precise extraction of relevant microstructure information, and new homogenization techniques allow the description and more reliable computation of effective properties. For homogenization approaches based on statistical first-, second-, and higher-order techniques, see, e.g., Eshelby (1957), Kröner (1977), Willis (1977), Torquato (2002), Adams et al. (2013) and Bacca et al. (2013a, 2013b). However, in order to exploit the maximum design potential of multiphase materials, inverse design methodologies, e.g., Ashby (2010), Adams et al. (2013), or Lobos and Böhlke (2015), are needed. This methodologies provide different strategies in the areas of, e.g., the screening of material data bases for attractive material candidates and combinations as well as the description of influence microstructure variation and its limitations (referred to as "properties closure" in Adams et al. (2013)) and, finally, for computing the best possible microstructure influence delivering properties as close as possible to the desired ones. This is significantly more powerful and structured than empirical techniques relying on experimental measurements and interpolation of the measured data since an infinite number of microstructures with possibly better properties will never be tested.

One small, however, important step in inverse design methodologies is the screening for materials which, in principle, inhibit the potential to offer the prescribed properties. This is not only crucial from a design point of view but is, as well, important information which can be easily included in local and online material data bases, e.g., https://www.materialsproject.org/, see e.g., Jain et al. (2013), de Jong et al. (2015) and Cheng et al. (2015). The principal limits of the anisotropic linear elastic material behavior of a multiphase material are described by their zeroth-order bounds. Unlike first- and second-order bounds of tensorial material properties, which need, respectively, one- and two-point statistical information of the microstructure, the zeroth-order bounds can be calculated without any statistical information. They require solely the

* Corresponding author. Tel.: +49 72160846900; fax: +49 72160844187.
E-mail addresses: mauricio.lobos@kit.edu (M. Lobos), thomas.boehlke@kit.edu (T. Böhlke).

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material constants of the constituents of the multiphase material. This information is sufficient in order to energetically enclose the effective material behavior of all realizations of the multiphase material, from above and from below, independently of the complexity and diversity of the real microstructure. This property makes the zeroth-order bounds perfect design descriptors for the physically motivated material screening. Naturally, further non-physical characteristics are important for the industrial design, as extensively discussed in Ashby (2010).

In the present work, the algorithm presented in Nadeau and Ferrari (2001) is reviewed and corrected, since the algorithm delivers indefinite tensors for specific positive definite stiffness tensors. A simple analytic example for this undesirable property is presented. The problem is solved by defining the lower bound through the dual operator and its upper bound. This ensures the positive definiteness of all zeroth-order bounds. Further, an alternative scalar anisotropy descriptor, which is invariant by consideration of the inverse tensors, is introduced, reflecting the anisotropy of a single anisotropic or a multiphase material. Further, in the present work, novel optimal bounds of the effective stiffness components are derived. The results are then applied to an exemplary material data base in order to illustrate the practical use.

In Section 2, the zeroth-order bounds and the algorithm of Nadeau and Ferrari are recapitulated. Then in Section 3, the corrected formulation is presented, together with the application on an exemplary data base. Conclusions are discussed in Section 4. The derivation of the optimal bounds for non-diagonal components is sketched in Appendix A. A simple example and a *Mathematica*® code of the algorithms are given in Appendix B and Appendix C, respectively.

Notation: A direct tensor notation is preferred throughout the text. Scalars are denoted by light-face type characters, e.g., a, b, α, β, W. First-order tensors are denoted by bold-face type lower case Latin characters, e.g., $\boldsymbol{x}, \boldsymbol{y}$. Second-order tensors are denoted by bold upper case Latin characters and Greek characters, e.g., $\boldsymbol{A}, \boldsymbol{\sigma}, \boldsymbol{\varepsilon}$. Fourth-order tensors are denote by blackboard bold upper case Latin characters, e.g., $\mathbb{C}, \mathbb{S}$. The Kronecker symbol is denoted by δ_{ij}. The scalar product between first- and second-order tensors is denoted as $\boldsymbol{a} \cdot \boldsymbol{b}$ and $\boldsymbol{A} \cdot \boldsymbol{B}$, respectively. Ortho-normal basis vectors $\boldsymbol{e}_i$, i.e., $\boldsymbol{e}_i \cdot \boldsymbol{e}_j = \delta_{ij}$, are used to describe all tensors. The tensor product is denoted by $\otimes$. The components of any tensor in respect to its ortho-normal basis are denoted by a_i, A_{ij}, C_{ijkl}, respectively for first-, second- and fourth-order tensors with the corresponding bases $\{\boldsymbol{e}_i\}$, $\{\boldsymbol{e}_i \otimes \boldsymbol{e}_j\}$ and $\{\boldsymbol{e}_i \otimes \boldsymbol{e}_j \otimes \boldsymbol{e}_k \otimes \boldsymbol{e}_l\}$. The identity on symmetric second-order tensors is denoted by $\mathbb{I}^S$ and has the components $I^S_{ijkl} = (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})/2$. A stiffness tensor $\mathbb{C}$ is a positive definite fourth-order tensor with minor and major symmetries, i.e., $C_{ijkl} = C_{jikl} = C_{klij}$. The trace of a stiffness tensor is defined as $\mathrm{tr}(\mathbb{C}) = C_{ijkl} I^S_{ijkl}$, where the Einstein's summation convention is applied. The linear map of a second-order tensor over a fourth-order tensor is denoted by $\mathbb{C}[\boldsymbol{\varepsilon}]$. A quadratic form $\boldsymbol{\varepsilon} \cdot \mathbb{C}[\boldsymbol{\varepsilon}]$ is computed as $\varepsilon_{ij} C_{ijkl} \varepsilon_{kl}$, where the Einstein's summation convention is applied. The inverse of a stiffness tensor on symmetric second-order tensors is denoted by $\mathbb{C}^{-1}$. The ensemble average of a quantity ψ is denoted as $\langle \psi \rangle$, which for ergodic media and the existence of a representative volume element V is calculated as $\int_V \psi \, \mathrm{dV/V}$. Effective quantities are denoted by a bar, e.g., $\bar{\psi}$.

2. Zeroth-order bounds

2.1. Definition

We consider an anisotropic linear elastic material behavior of a multiphase material without pores or cracks for statistical homogeneous and ergodic media. The existence of a representative volume element V is assumed. In this case, the microscopic and effective material laws are given by

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \mathbb{C}(\boldsymbol{x})[\boldsymbol{\varepsilon}(\boldsymbol{x})] \qquad \boldsymbol{x} \in V \ , \quad \bar{\boldsymbol{\sigma}} = \bar{\mathbb{C}}[\bar{\boldsymbol{\varepsilon}}] \ , \tag{1}$$

with the symmetric Cauchy stress tensor $\boldsymbol{\sigma}$, the infinitesimal strain tensor $\boldsymbol{\varepsilon}$, and the effective measures $\bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma} \rangle$ and $\bar{\boldsymbol{\varepsilon}} = \langle \boldsymbol{\varepsilon} \rangle$, respectively, see Hill (1952). The effective anisotropic linear elastic material behavior $\bar{\mathbb{C}}$ connects the effective strains and stresses and depends on the material constituents (phases) and the underlying microstructure (volume fractions, morphology, etc.). In case of a scale separation, the effective stiffness is independent of the boundary conditions applied to the representative volume element.

Statistical bounds can be formulated in order to enclose the effective material behavior by energy principles and consideration of some limited amount of statistical information. An elasticity tensor is called a bound if the material behavior of all realizations lies energetically below or above of this tensor. The earliest bounds were formulated by Voigt (1910) and Reuss (1929). They are first-order bounds since they require one-point statistical information, i.e., volume fractions. These bounds enclose the effective material behavior from above and below, describing a region where the material behavior of all realizations of the considered materials is included. This region reflects, in principle, the design variability offered by the chosen materials. The explicit calculation of all one-point statistics for multiple arbitrarily anisotropic materials is, however, a complex task if information of design possibilities of a single material or of multiphase materials is desired. The zeroth-order bounds offer a simple approach for the fast identification of the design options of a material with arbitrary anisotropy and number of phases. It should be stressed that this set is larger than the set enclosed by the first- and higher-order bounds, i.e., the set enclosed by the zeroth-order bounds contains trivially the sets enclosed by all higher-order bounds, see Lobos and Böhlke (2015) for examples for cubic materials.

The zeroth-order bounds are formulated as the tensors which enclose the effective elastic energy density

$$\bar{W} = \frac{1}{2} \bar{\boldsymbol{\varepsilon}} \cdot \bar{\mathbb{C}}[\bar{\boldsymbol{\varepsilon}}], \tag{2}$$

from above and below, i.e.,

$$\bar{\boldsymbol{\varepsilon}} \cdot \mathbb{C}^-[\bar{\boldsymbol{\varepsilon}}] \le \bar{\boldsymbol{\varepsilon}} \cdot \bar{\mathbb{C}}[\bar{\boldsymbol{\varepsilon}}] \le \bar{\boldsymbol{\varepsilon}} \cdot \mathbb{C}^+[\bar{\boldsymbol{\varepsilon}}] \quad \forall \bar{\boldsymbol{\varepsilon}} \ , \tag{3}$$

independently of the microstructure arrangement. In the following, this kind of inequalities between quadratic forms will be noted shortly as

$$\mathbb{C}^- \le \bar{\mathbb{C}} \le \mathbb{C}^+. \tag{4}$$

An important consequence of this inequalities is that the main components of the effective material behavior are enclosed as follows (no summation)

$$C^-_{\alpha\alpha} \le \bar{C}_{\alpha\alpha} \le C^+_{\alpha\alpha} \quad \alpha \in \{11, 22, 33, 23, 13, 12\}. \tag{5}$$

All other components (non-diagonal components) can also be enclosed if the fourth-order tensor is considered as a matrix. In Proust and Kalidindi (2006), degenerated bounds of the non-diagonal components are presented. These bounds are correct, are, however, not the best possible bounds since they are not optimal. In Appendix A, the derivation of the optimal bounds of non-diagonal components is presented, which are

$$\begin{aligned} &\Gamma^-_{\alpha\beta} \le \bar{C}_{\alpha\beta} \le \Gamma^+_{\alpha\beta} \quad \alpha \neq \beta \in \{11, 22, 33, 23, 13, 12\}, \\ &\Gamma^-_{\alpha\beta} = \mu_{\alpha\beta} - \frac{1}{2}\sqrt{\Delta_\alpha \Delta_\beta} \ , \quad \Gamma^+_{\alpha\beta} = \mu_{\alpha\beta} + \frac{1}{2}\sqrt{\Delta_\alpha \Delta_\beta}, \\ &\mu_{\alpha\beta} = \frac{1}{2}(C^-_{\alpha\beta} + C^+_{\alpha\beta}) \ , \quad \Delta_\alpha = C^+_{\alpha\alpha} - C^-_{\alpha\alpha}. \end{aligned} \tag{6}$$