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Research paper

Consideration of arbitrary inclusion shapes in the framework of isotropic continuum micromechanics: The replacement Eshelby tensor approach

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ABSTRACT

The effective behavior of matrix-inclusion materials is governed by the properties and volume fractions of involved material phases as well as by the morphology of the inclusion domain. Eshelby's solutions on the ellipsoidal inclusion problem (Eshelby, 1957) paved the way to the development of a vast number of continuum micromechanics based homogenization schemes for evaluation of effective properties. This paper proposes an approach for utilizing these homogenization schemes also for non-ellipsoidal inclusions with particular focus on macroscopic isotropy. The key concept is to replace the originally-used Eshelby tensor by an analogous representation capturing the effect of non-spherical inclusions on strain fluctuation within the material domain. The so-called replacement Eshelby tensor is obtained by numerical evaluation of two adjustment factors being functions of the inclusion morphology and the stiffness contrast between the matrix and inclusion phase. These factors are evaluated and discussed for selected inclusion morphologies. Finally, the replacement Eshelby tensor approach is implemented in a homogenization procedure for effective elastic properties (cascade continuum micromechanics model (Timothy and Meschke, 2016)) as well as in a scheme for determining effective yield surfaces in case of plastic material behavior (Traxl and Lackner, 2015).

1. Introduction

Inhomogeneities in materials strongly affect various physical properties such as elasticity, viscosity, strength, diffusivity, and conductivity. The effective material behavior results not only from the volume fractions and properties of the involved material phases, but also from their spatial arrangement and morphology. Considering volume fractions and properties of constituents while disregarding the actual morphology of material phases merely allows a rough confinement of potential effective properties by the Reuss–Voigt upper and lower bounds (Reuss, 1929; Voigt, 1889). This range of potential effective properties can be narrowed by assuming macroscopic isotropy, yielding the Hashin–Shtrikman bounds (Hashin and Shtrikman, 1963). Still, the range between upper and lower bound may be considerable – especially for high contrasts of properties between the involved material phases (e.g., the lower bound of the Hashin–Shtrikman estimate yields zero stiffness for porous materials even for low porosities) – highlighting the significance of considering the morphology of materials for an improved prediction of effective properties.

In his fundamental work, Eshelby (1957) provided solutions for ellipsoidal inclusions, allowing the assessment for stress and strain fluctuations provoked by an individual inhomogeneity in the course of loading. This solution is an integral part of subsequently developed continuum micromechanics-based homogenization schemes – most notably, the *dilute scheme* (cp., e.g., Zaoui (2002)), the *differential scheme* (Norris, 1985), the *self-consistence scheme* (Hill, 1965), and the *Mori–Tanaka scheme* (Mori and Tanaka, 1973; Benveniste, 1987). More recently, these approaches were extended towards plasticity (e.g., Dormieux et al. (2006); Zhou and Meschke (2014); Traxl and Lackner (2015)) and viscoelasticity (e.g., Laws and McLaughlin (1978); Pichler and Lackner (2008); Dinzart and Lipiński (2010) utilizing the correspondence principle (Lee, 1955)). In the *cascade continuum micromechanics model* (Timothy and Meschke, 2016), an additional parameter associated with the microstructure morphology is introduced, yielding the aforementioned micromechanics-based homogenization schemes as special cases. While this morphology parameter accounts for the connectivity of the matrix for high volume fractions of inclusions, the cascade model – and, hence, all above mentioned schemes – converge to the dilute scheme for low volume fractions of inclusions, with the latter considering the aspect ratios of the ellipsoidal inclusions while disregarding the interaction between inclusions.

For capturing non-ellipsoidal inclusions while still utilizing continuum micromechanics-based methods to account for the interaction between inclusions, semi-analytical approaches were presented in

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Bradshaw (2003) and Duschlbauer et al. (2006). Therein, the average of strain concentration within an inclusion induced by a constant far-field strain state was determined in finite element simulations and implemented in the Mori–Tanaka scheme. Beyond elasticity, this approach, referred to as the *replacement Mori–Tanaka method* (RMTM), was also applied for modeling conductivity and the thermomechanical behavior of diamond reinforced composites (Nogales and Böhm, 2008). In another semi-analytical approach, the influence of a single inclusion is captured in terms of numerically evaluated *compliance/stiffness contribution tensors* (see, e.g., Tsukrov and Novak (2002)) while the interaction between inclusions is considered analytically (Sevostianov and Kachanov, 2007; Eroshkin and Tsukrov, 2005; Drach et al., 2016).

Alternatively, the effect of individual inclusions and their interaction can be captured at once by direct numerical simulations ranging from the modeling of unit cells (e.g., Meijer et al. (1997)), randomly generated volume elements (e.g., Shen and Lissenden (2005); Galli et al. (2008); Fritzen and Böhlke (2011)) to the analysis of geometries obtained from tomography (e.g., Terada and Kikuchi (1996); Macneil and Boyd (2008)) or electron microscopy (Gudlur et al., 2014). Direct finite element simulations in Rasool and Böhm (2012) revealed a pronounced influence of inclusion shapes on the stress field within the inclusions. In Böhm and Rasool (2016), the numerical approach was extended towards non-linear material behavior for considering the influence of the inclusion shape on the effective thermoelastoplastic properties of composites. For a comparison of different homogenization approaches, see Klusemann et al. (2012).

Inspired by Bradshaw (2003) and other contributions mentioned above, the present paper accounts for non-ellipsoidal inclusions by combining methods of continuum micromechanics with the numerical computation of the effective impact of a single inclusion. The key concept outlined in this paper is to replace Eshelby's solution for ellipsoidal inclusions (i.e., the *Eshelby tensor*) by an appropriate analogon, subsequently called *replacement Eshelby tensor* in analogy to the term *replacement strain concentration tensor* used in the RMTM (Nogales and Böhm, 2008). This approach allows a straight forward extension of existing Eshelby-based linear and non-linear homogenization procedures. While the concept is basically applicable to the general case of anisotropy, the present paper focuses on macroscopically isotropic material behavior, reducing the Eshelby tensor and, hence, the replacement Eshelby tensor to two scalars associated with the volumetric and deviatoric material response.

The paper is organized as follows: After recalling the inclusion problem in continuum micromechanics and implications of Eshelby's solution, the replacement Eshelby tensor concept is presented in Section 2. Subsequently, the applicability of the method is demonstrated in Section 3 for elastic and plastic homogenization problems considering selected inclusion shapes with special focus on pores and rigid inclusions. Finally, a summary and conclusions are given in Section 4.

2. Method

As the basic outcome, Eshelby (1957) provided a solution for the resulting strain field in a homogeneous material loaded by a pre-strain within an ellipsoidal subdomain. A fundamental idea of continuum micromechanics-based homogenization schemes is to use this solution to express strain fluctuations induced by inhomogeneities by introducing equivalent pre-strains in a fictitious homogeneous material resulting in an *equivalent eigenstrain field*. This principle is recapitulated first in this section in order to highlight the differences between ellipsoidal and non-ellipsoidal inclusions. Based on this, the replacement Eshelby tensor concept is introduced thereafter.

2.1. Homogenization

Consider a spatial domain Ω of a material with volume V constituting a *representative elementary volume* (REV) as satisfying the *separation of scales condition* (Hashin, 1983). Accordingly, the size of Ω is significantly larger than the characteristic length of inhomogeneities but significantly smaller than the characteristic distance of load induced macroscopic stress/strain fluctuations (i.e., fluctuations that would also occur if the material was homogeneous). Inhomogeneities induce additional local fluctuations within Ω leading to spatially varying stress and strain fields, $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$. The average of these quantities are referred to as the *effective stress* and *effective strain*, respectively:

$$\boldsymbol{\Sigma} = \langle\boldsymbol{\sigma}\rangle_\Omega = \frac{1}{V}\int_\Omega \boldsymbol{\sigma}(\mathbf{x})\,d\mathbf{x}\ , \quad \mathbf{E} = \langle\boldsymbol{\varepsilon}\rangle_\Omega = \frac{1}{V}\int_\Omega \boldsymbol{\varepsilon}(\mathbf{x})\,d\mathbf{x}\ , \tag{1}$$

where $\langle\bullet\rangle_\Omega$ denotes the averaging operator applied on the domain Ω. Reversely, the respective local values can be obtained with *stress* and *strain concentration tensors*:

$$\boldsymbol{\sigma}(\mathbf{x}) = \mathbb{B}(\mathbf{x}) : \boldsymbol{\Sigma}\ , \quad \boldsymbol{\varepsilon}(\mathbf{x}) = \mathbb{A}(\mathbf{x}) : \mathbf{E}\ . \tag{2}$$

The goal of homogenization is finding the constitutive relation between the $\boldsymbol{\Sigma}$ and $\mathbf{E}$ departing from local material properties.

2.2. Equivalent eigenstrain principle

In an inhomogeneous material with spatially varying elastic properties, the constitutive relation in a material point $\mathbf{x}$ is given by

$$\boldsymbol{\sigma}(\mathbf{x}) = \mathbb{C}(\mathbf{x}) : \boldsymbol{\varepsilon}(\mathbf{x}) \tag{3}$$

with $\mathbb{C}$, $\boldsymbol{\sigma}$, and $\boldsymbol{\varepsilon}$, respectively, denoting the local elasticity, stress, and strain tensor. The stress field resulting from Eq. (3) can equivalently be obtained by a substitution problem consisting of a homogeneous reference material characterized by a constant elasticity tensor $\mathbb{C}_0$ and loaded by a spatially varying pre-strain $\boldsymbol{\varepsilon}^*$:

$$\boldsymbol{\sigma}(\mathbf{x}) = \mathbb{C}_0 : (\boldsymbol{\varepsilon}(\mathbf{x}) - \boldsymbol{\varepsilon}^*(\mathbf{x}))\ , \tag{4}$$

where

$$\boldsymbol{\varepsilon}^*(\mathbf{x}) = (\mathbb{C}_0^{-1} : \mathbb{C}(\mathbf{x}) - \mathbb{I}) : \boldsymbol{\varepsilon}(\mathbf{x})\ . \tag{5}$$

Considering materials consisting of discrete numbers of homogeneous material phases (i.e., material properties are spatially constant within each phase), occupying the spatial domain Ω_α (the index α refers to the respective material phase), Eq. (5) becomes

$$\boldsymbol{\varepsilon}^*(\mathbf{x}) = -\mathbb{H} : \boldsymbol{\varepsilon}(\mathbf{x}) \quad \text{for} \quad \mathbf{x} \in \Omega_\alpha \tag{6}$$

with

$$\mathbb{H} = (\mathbb{C}_0^{-1} : \mathbb{C}_\alpha - \mathbb{I})\ . \tag{7}$$

2.3. Inclusion problem

Substituting the heterogeneous formulation in Eq. (3) by the equivalent eigenstrain formulation in Eqs. (4) and (6) raises two major problems:

(i) In reference to Eq. (4): How does $\boldsymbol{\varepsilon}^*$, occurring within Ω_α, effect the strain field within a homogeneous material?
(ii) In reference to Eq. (6): What is the actual strain field $\boldsymbol{\varepsilon}$ within Ω_α induced by external loading of a heterogeneous material?

These two problems are commonly known as the (i) *homogeneous* and (ii) *inhomogeneous inclusion problem* (Ma and Korsunsky, 2014), or,