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A micromechanics approach to homogenizing elasto-viscoplastic heterogeneous materials

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ABSTRACT

The variational asymptotic method for unit cell homogenization (VAMUCH) has emerged as a general-purpose micromechanics code capable of predicting the effective properties of heterogeneous materials and recovering the local fields. The objective of this paper is to propose a micromechanics approach enabling VAMUCH to homogenize elasto-viscoplastic heterogeneous materials. An affine formulation of the constitutive relations for an elasto-viscoplastic constituent, which exhibits viscoplastic anisotropy and combined isotropic–kinematic hardening, is derived. The weak form of the problem is derived using an asymptotic method, discretized using finite elements, and implemented into VAMUCH. The new features of VAMUCH are validated with examples such as homogenizing binary, fiber-reinforced, and particle-reinforced composites. VAMUCH is found to be capable of handling various microstructure, complex material models, complex loading conditions, and complex loading paths. More sophisticated material models can be implemented into it.

1. Introduction

Heterogeneous materials are widely used in structural components due to their capabilities of exhibiting designated in-plane stiffness, bending stiffness, ultimate strength, or thermal expansion coefficient. When they are deformed to certain extents at high temperatures, their constituents often exhibit elasto-viscoplastic behaviors. It is challenging to evaluate their mechanical responses because their deformations are often accompanied by material nonlinearity, history dependency, and rate dependency. Moreover, it is difficult and time consuming to manufacture a great amount of specimens and to perform various tests on them, while it is computationally prohibitive to analyze them with all the microstructural details because the dimensions of the macroscopic structures are usually several orders of magnitude greater than the heterogeneity length scale. Therefore, it is of great practical value to solve such problems using a micromechanics approach.

In recent decades, numerous efforts have been devoted to micromechanics. A micromechanics approach generally consists of the following steps (Yu and Tang, 2007a):

1. Identify the unit cell (UC) of a heterogeneous material.
2. Compute the effective material properties through the constitutive modeling of the UC.
3. Assign these properties to the macroscopic structure and obtain the global response.
4. Feedback the global response to the local scale and recover the local fields (e.g., the displacement, strain, and stress fields).

If the deformation is restricted in the linearly elastic regime it is history- and rate-independent. In this case, the effective material properties remain constant all the time, and one just needs to perform the constitutive modeling. The micromechanics theories of linearly elastic heterogeneous materials are well established. These theories include the mean-field homogenization (MFH) (Hill, 1965a; Mori and Tanaka, 1973), Hashin and Shtrikman's variational approach (Hashin and Shtrikman, 1963), the third-order bounds (Milton, 1981), the method of cells (MOC) (Aboudi, 1981), the recursive cell method (Banerjee and Adams, 2004), and the mathematical homogenization theories (MHT) (Bensoussan et al., 1978; Murakami and Toledano, 1990), and some others. If the deformation is extended to the viscoplastic regime, it becomes history- and rate-dependent. In this case, there does not exist a correspondence principal between the stress and strain rates, and one must linearize the constitutive relations and perform an incremental analysis.

MFH is among the most popular micromechanics approaches and consists of two major approaches, i.e., the tangent and secant

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approaches. As the name suggests, the tangent approach is based on a tangent linearization of the constitutive relations (Hill, 1965b; Lebensohn and TomT, 1993), while the secant approach is based on a secant linearization (Berveiller and Zaoui, 1978; Tandon and Weng, 1988; Suquet, 1995). Hutchinson (1976) first enabled Hill's incremental approach to homogenize rigid-viscoplastic polycrystals. Weng (1982) proposed a secant approach to homogenizing elasto-viscoplastic polycrystals, in which the inelastic strain is treated as a stress-free eigenstrain such that the problem is transformed to an elastic one. Nemat-Nasser and Obata (1986) later improved this approach by taking account into finite deformation. These early approaches are unable to take account into the viscoplastic interactions among different constituents and tend to generate too stiff predictions.

Elaborate efforts have been devoted to overcoming these drawbacks. Li and Weng (1998) improved the secant approach by transforming the problem to a viscoelastic one, while Molinari et al. (1987, 1997) improved the tangent approach by transforming the problem to a thermoelastic one. Despite improvements, these two approaches either require a two-phase heterogeneous material or tend to underestimate the flow stress. Masson and his coworkers (Masson and Zaoui, 1999; Masson et al., 2000) proposed an affine approach, in which the constitutive relations are first linearized in the time domain and then transformed to the Laplace domain such that the problem is transformed to a thermoelastic one, and Pierard and his coworkers (Pierard and Doghri, 2006; Pierard et al., 2007) later enabled this approach to handle two-phase heterogeneous materials. Although the affine approach is capable of generating close predictions, it requires the inverse Laplace transformation, which is computationally costly. To overcome this drawback, Doghri et al. (2010) proposed an incrementally affine approach, in which the constitutive relations are linearized in numerous discrete time intervals such that the inverse Laplace transformation is avoided. Despite success, none of the aforementioned approaches can either recover the local fields or incorporate viscoplastic anisotropy and combined isotropic–kinematic hardening. Therefore, there is a need for a more powerful approach.

Numerous attempts have been made not only to linearize the constitutive relations but also to recover the local fields. Aboudi and his co-workers (Aboudi, 1982; Paley and Aboudi, 1992) developed the method of cells (MOC) and later the generalized method of cells (GMC) to achieve this goal. A detailed review on these approaches can be found in Adoudi (2004). The basic ideas of these approaches include subdividing the UC into numerous cuboid subcells, solving for the average strains and stresses over each subcell, and estimating the local fields. Despite improvements, these approaches suffer two major drawbacks: first, discretizing the UC using cuboid subcells may introduce considerable domain approximation errors; second, approximating the local fields using the average local strains and stresses may introduce considerable approximation errors. In fact, it is always more accurate to discretize the UC using a finite element mesh and to approximate the local fields using shape functions and nodal values. To overcome these drawbacks, Aboudi et al. (2002) developed the high fidelity generalized method of cells (HFGMC). Despite high accuracy, HFGMC is found to be quite computationally costly (Williams et al., 2007). All these lead one to seek for a more accurate and efficient approach.

In recent years, Yu and his co-workers (Yu and Tang, 2007a,b; Tang and Yu, 2007, 2008a,b) developed the variational asymptotic method for unit cell homogenization (VAMUCH). VAMUCH is a general-purpose micromechanics code capable of predicting the effective material properties and recovering the local fields. One of its unique features is that it has the minimum number of assumptions:

1. The heterogeneous material can be homogenized.
2. The effective material properties of a UC are independent of the geometry and boundary conditions of the macroscopic structure.

These two assumptions place the fewest restrictions on problem solving. Although VAMUCH seems as versatile as the traditional finite element method (FEM), it is distinct to FEM at least in the following aspects:

1. VAMUCH is specially developed for the constitutive modeling, while FEM is not, or to say, VAMUCH directly solves for the constitutive relations, while FEM directly solves for the displacements, strains, and stresses under certain load conditions.
2. VAMUCH can model the UC using the smallest mathematical building block, not necessarily a 3D volume, while FEM cannot (e.g., VAMUCH can use 1D and 2D UCs to compute the complete set of 3D properties of binary and fiber-reinforced composites, respectively (Yu and Tang, 2007a), while FEM has to use 3D UCs to achieve this).
3. VAMUCH solves for the fluctuation functions (see Eq. (49)), while FEM solves for the displacements.
4. VAMUCH deals with periodic boundary conditions, while FEM mostly deals with displacement and traction boundary conditions.
5. VAMUCH can obtain the complete set of effective material properties through one analysis, while FEM cannot (e.g., for linearly elastic materials, FEM has to run six times to do this (Xia et al., 2003)).

The objective of this paper is to propose a micromechanics approach enabling VAMUCH to homogenize elasto-viscoplastic heterogeneous materials. An affine formulation of the constitutive relations for an elasto-viscoplastic constituent, which exhibits viscoplastic anisotropy and combined isotropic–kinematic hardening, is derived. The weak form of the problem is derived using an asymptotic method, discretized using finite elements, and implemented into VAMUCH. The new features of VAMUCH are validated with examples such as homogenizing binary, fiber-reinforced, and particle-reinforced composites.

2. Thermodynamic formulations

Consider a heterogeneous material of an identifiable UC. Without loss of generality, let its constituents all be elasto-viscoplastic. Note that an elastic constituent can be treated as an elasto-viscoplastic one with infinite yield stress. In this section, some fundamentals of thermodynamics will be briefed.

Let ψ denote the Helmholtz free energy per unit mass of the constituent. According to the theory of thermodynamics, ψ can be expressed as a function of a suitable set of independent state variables characterizing the elastic and viscoplastic behaviors of the constituent, e.g.,

$$\psi = \psi(\boldsymbol{\epsilon}^e, \boldsymbol{\alpha}, r), \tag{1}$$

where $\boldsymbol{\epsilon}^e$ denotes the elastic strain tensor, $\boldsymbol{\alpha}$ is a second-order tensor accounting for kinematic hardening, and r is a scalar accounting for isotropic hardening. Assume that the constituent exhibits uncoupled elastic and viscoplastic behaviors. In this case, ψ can be decomposed into its elastic part, ψ^e, and its hardening part, ψ^{vp}, i.e.,

$$\psi(\boldsymbol{\epsilon}^e, \boldsymbol{\alpha}, r) = \psi^e(\boldsymbol{\epsilon}^e) + \psi^{vp}(\boldsymbol{\alpha}, r). \tag{2}$$

The thermodynamic forces conjugate to the state variables in Eq. (1) can be defined as