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Micromechanics of inelastic composites with misaligned inclusions: Numerical treatment of orientation

Issam Doghri [a,*], Laurent Tinel [b]

[a] Université Catholique de Louvain (UCL), CESAME, Bâtiment Euler, 4 Avenue G. Lemaître, B-1348 Louvain-la-Neuve, Belgium
[b] e-Xstream engineering SA, 4 Avenue A. Einstein, B-1348 Louvain-la-Neuve, Belgium

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Paper dedicated to Professor Thomas J.R. Hughes on the occasion of his 60th birthday

Abstract

This paper is concerned with the micromechanics of multi-phase fiber- or inclusion-reinforced inelastic composites with a special emphasis on the numerical treatment of misaligned orientation. Mean-field homogenization of these composites involves volume and orientation averaging. The latter usually needs average orientation measures known as the second- and fourth-rank orientation tensors $\boldsymbol{a}$ and $\boldsymbol{A}$, respectively. Usually the only orientation data available is $\boldsymbol{a}$ and a first issue is to reconstruct $\boldsymbol{A}$ using closure approximations. We propose a new weighted regularization method which deals with orientations which are strictly neither 1D, 2D nor 3D and ensures a smooth transition between the 3 cases. A second issue is that there are situations where the inclusions' orientation distribution function (ODF) is needed for homogenization but is unavailable. The ODF is recovered using $\boldsymbol{a}$ and $\boldsymbol{A}$ and numerically computed at a number of discrete orientations. A third issue is the actual computation of orientation averaging integrals. An efficient algorithm approximates the integrals with sums over a finite number of orientations. Orientation and volume averaging concepts are applied to the mean-field homogenization of two classes of multi-phase composites: linear thermo-elastic and rate-independent inelastic. In the latter case, an incremental formulation is proposed which enables the simulation of unloading, cyclic and otherwise non-proportional loadings. Implicit time-discretization and consistent tangent operators are employed. The procedures and the corresponding algorithms were implemented in the [DIGIMAT version 1.4, 2004. Linear and nonlinear multi-scale material modeling software, e-Xstream engineering SA (http://www.e-Xstream.com), Louvain-la-Neuve, Belgium.] software and several numerical simulations show their accuracy and efficiency.

Keywords: Composites; Micromechanics; Homogenization; Orientation distribution function; Orientation tensors; Inelasticity

* Corresponding author. Tel.: +32 10 478042/472350; fax: +32 10 472180.
E-mail addresses: doghri@mema.ucl.ac.be (I. Doghri), laurent.tinel@e-xstream.com (L. Tinel).

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1. Introduction

Fiber- or inclusion-reinforced composite materials enjoy a wide use in various industries. The modern way to model them is via multi-scale or micro–macro methods which predict the influence of the microstructure on the macroscopic properties. Scale-transition methods for these composites can be classified into four categories.

(1) Direct finite element (FE) simulations of a unit cell (assuming periodic microstructures) or a representative volume element (RVE). A pioneering contribution was made by Adams [3] who realized transverse load simulations of an elasto-plastic matrix reinforced with long and aligned elastic fibers. A large number of other papers followed, e.g., [31,58,8,51,32,49,11,30].
(2) Transformation field analysis or subcell method (where a unit cell or a RVE is subdivided into a number of 2D pixels or 3D voxels); see [23,2,6,48,27]. The latter authors subdivided each cell into 4 subcells and enforced traction and strain compatibility in terms of average stresses and strains in each subcell.
(3) Homogenization based on asymptotic expansion of the displacement field (it assumes a periodic microstructure and ends up with a unit cell problem to be solved by FE); examples are [35,31].
(4) Mean-field homogenization based on assumed relations between average values of microstrain and stress fields in each phase; examples are [55,36,47,42,26,45,19,18,43].

In this paper, we study the latter scale transition method. There are several phenomena it is unable to describe (clustering, percolation, strain localization and size effects—except when combined with a Hall–Petch-type model) and for homogenization models based on the Eshelby [24] results, the inclusions' shape can only be ellipsoidal. However, when the conditions of their application are met, and when one is interested only in the effective properties and the per-phase averages of stress and strain, mean-field homogenization models provide by far the most cost-effective solution (in terms of computer time and also ease-of-use). The models have been applied with success to a large variety of composites based on polymer, metal, ceramic or concrete matrices.

Most of the literature on micro–macro modeling of composites (including the above-mentioned references) deals with fixed orientation fibers or orientation-irrelevant spherical inclusions, while this paper deals with multi-phase composites. These are such that a matrix material is reinforced with multiple phases of misaligned inclusions. Each inclusion is supposed to be a spheroid (that is an ellipsoid of revolution) with unit axis vector $\boldsymbol{p}$ and aspect ratio $A_r > 0$ (boldface symbols denote tensors or matrices, the rank of which is indicated by the context). Fibers and platelets can be approximated with prolate ($A_r > 1$) and oblate ($A_r < 1$) spheroids, respectively.

Mean-field homogenization of such multi-phase composites has been studied in linear thermo-elasticity (e.g., [10,22,44]) and elasto-plasticity (e.g., [21,20]). However, some important issues related to the numerical treatment of misaligned inclusions' orientation have not been addressed and it is the objective of the present paper to study them.

A first issue is that the inclusions' orientation distribution function (ODF) $\psi(\boldsymbol{p})$ is usually unavailable (e.g., injection molding of short fiber reinforced polymer composites). The only information one has is a second-rank orientation tensor $\boldsymbol{a}$ which is the ODF-weighted average of $\boldsymbol{p} \otimes \boldsymbol{p}$ (the symbol $\otimes$ designates a tensor or dyadic product). However, in the computation of effective stiffness operators, one needs a fourth-rank orientation tensor $\boldsymbol{A}$ which is the ODF-weighted average of $\boldsymbol{p} \otimes \boldsymbol{p} \otimes \boldsymbol{p} \otimes \boldsymbol{p}$. An important problem is to approximate $\boldsymbol{A}$ from $\boldsymbol{a}$. This is the subject of closure approximations. We propose a new weighted formula for cases (most often encountered in practice) where the orientation is strictly neither 2D nor 3D. Numerical simulations show that unless the new weighted scheme is used, unrealistic predictions can be obtained in some instances.