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Pseudo-grain discretization and full Mori Tanaka formulation for random heterogeneous media: Predictive abilities for stresses in individual inclusions and the matrix

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ABSTRACT

Both effective properties of composite and the stresses in the individual inclusions and in the matrix are necessary for modelling damage in short fibre composites. Mean field theorems are usually used to calculate the effective properties of composite materials, most common among them is the Mori–Tanaka formulation. Owing to occasional mathematical and physical admissibility problems with the Mori–Tanaka formulation, a pseudo-grain discretized Mori–Tanaka formulation (PGMT) was proposed in literature. This paper looks at the predictive capabilities for stresses in individual inclusions and matrix as well as the average stresses in inclusion phase for full Mori–Tanaka and PGMT formulation for 2D planar distribution of orientation of inclusions. The average stresses inside inclusions and the matrix are compared to solutions of full-scale finite element (FE) models for a wide range of configurations. It was seen that the Mori–Tanaka formulation gave excellent predictions of average stresses in individual inclusions, even when the basic assumptions of Mori–Tanaka were reported to be too simplistic, while the predictions of PGMT were off significantly in all the cases. The predictions of the matrix stresses by the two methods were found to be very similar to each other. The average value of stress averaged over the entire inclusion phase was also very close to each other. The Mori–Tanaka formulation must be used as the first choice homogenization scheme.

1. Introduction

Short fibre composites are a class of composite materials having short fibres randomly oriented in a resin. These materials are finding increasing relevance as semi-structural components in the automotive industry. Both effective properties and the stresses in the individual inclusions and in the matrix are necessary for modelling damage events like fibre matrix debonding and fibre breakage in short fibre composites. The effective properties of composites can be estimated by a number of methods, most common among them are the mean field homogenization schemes. Almost all mean field homogenization schemes are based on the work of Eshelby [1]. The most popular among them was developed by Mori and Tanaka [2]. When the formulation of Eshelby and consequently Mori and Tanaka are applied to short fibre composites, fibres are modelled as ellipsoidal inclusions. Thus the terms, “fibre” and “inclusion” are generally used interchangeably in the context of homogenization of short fibre composites.

Effective stiffness of a composite is usually calculated by relating the strain concentration factor of the inclusions to the effective stiffness of a composite by the relation:

$$C^{eff} = C^m + \sum_{\alpha=1}^{M} c_\alpha (C^\alpha - C^m) A^\alpha \tag{1}$$

where C^{eff} is the effective stiffness of the composite, C^m, C^α are the stiffness matrix of the matrix and inclusion respectively, c_α is the volume fraction of individual inclusion, M is the total number of inclusions and A^α is the strain concentration factor which relates the strain in the inclusion to the applied strain. A detailed mathematical description of the Mori–Tanaka formulation can be found in literature [3].

The Mori–Tanaka formulation is often criticized for giving physically inadmissible solutions. Benveniste et al., [4] proved that Mori–Tanaka and self-consistent schemes would always yield a symmetric effective stiffness tensor, only if the composite had reinforcements of similar shape and alignment. Weng [5] noticed that the Mori–Tanaka approach in multi-phase composites could

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violate the Hashin–Shtrikman bounds. The effective property of a composite at unitary (100%) reinforcement was shown by Ferrari [6] to be depending on spurious matrix properties, this was described as ‘‘physically unacceptable’’. It was concluded that the Mori–Tanaka formulation is suitable for composites with reinforcements of similar shape and orientation or if the distribution of orientation is statistically homogenous random. However, the Mori–Tanaka formulation is often used for multiphase composites having inclusions with a statistical distribution of length and orientation. It is this extension from two-phase composites to multi-phase composites and not the original Mori–Tanaka assumption that was said to occasionally produce physically inadmissible results.

Pierard et al. [7] proposed a method to circumvent the mathematical problems of the Mori–Tanaka formulation. They discretized the volume element (VE) to a number of ‘‘pseudo-grains’’. A pseudo-grain was defined as a bi-phase composite consisting of inclusions having the same orientation and aspect ratio. They applied the Mori–Tanaka formulation individually on the ‘‘pseudo-grains’’ and then volume averaged the stiffness of the grains to get the effective properties of the short-fibre composite. The basic idea behind breaking the homogenization scheme into two steps is the following: if each step individually satisfies all the conditions of the homogenization scheme, then the procedure in itself will satisfy all the conditions required for mean-field homogenization schemes. This approach eliminated the mathematical problems of the Mori–Tanaka formulation but introduced additional approximations with regard to the interactions between the inclusions. This idea of discretising the VE into several ‘‘pseudo-grains’’ was also implemented by Kaiser and Stommel [8]. We will call this ‘‘pseudo-grain’’ formulation of the Mori–Tanaka method in short the ‘‘PGMT’’ formulation.

There are a number of papers in literature describing comparisons of the predictions of the effective response of composite materials by various mean field theories with finite element simulations of microstructures. A few of them are Kari et al. [9], Gusav [10], Llorca et al. [11], Ghossein et al. [12] and Sun et al. [13]. A detailed review of different mean-field schemes for uni-directional short fibre composites can be found in [14]. A comparison between the predictions of effective response by the Mori–Tanaka formulation and PGMT formulation was done by Doghri and Tinel [15]. All the above articles [9–15] focused primarily on the comparison of predictions of effective mechanical properties of an VE. Average stresses in individual inclusions are required to model damage events like fibre matrix de-bonding and fibre failure [16], while the average stresses in the matrix are usually used to model the material non-linearity in the matrix. The predictions of average stresses in individual inclusions are as significant as the equivalent effective properties. For the case of non-aligned ellipsoidal inclusions, the micro-stresses in individual inclusions are a function of the orientation of the inclusion. Duschlbauer et al. [17] compared predictions of normalized maximum principal stresses in individual inclusions by a modified Mori–Tanaka formulation and FE results for a VE with 2D-planar uniform random arrangement of carbon fibres in a copper matrix. Barring this, there is limited literature validating the prediction of stresses in individual non-aligned ellipsoidal inclusions by the Mori–Tanaka formulation and to our knowledge none for PGMT.

In this paper, we compare the predictive abilities for stresses in individual inclusions and the matrix of the Mori–Tanaka formulation and the PGMT formulation with the finite element (FE) calculations. The predictions of the Mori–Tanaka and PGMT formulation are compared with the results of the FE simulations. A number of cases including fully aligned inclusions, non-aligned inclusions including approximations of 2D-planar uniform random, statistical distribution of orientations and different length distributions are considered. All the models considered in this paper had only a planar variation of orientation. The aspect ratio of inclusions in most of the cases is taken to be 3, while the volume fraction of inclusions varies from 0.01 to 0.25. Inclusions with aspect ratio 15 were modelled as sphero-cylinder. An applied load of 1% uniaxial strain is considered throughout the paper. Comparisons are made for both the stresses in the applied load direction, S11 as well as transverse loading direction, S22. All the stresses are calculated in the global co-ordinate system of the orientation tensor. Average stresses in individual inclusions are referred in the rest of the article as ‘‘inclusion average’’; while the average of stresses across all inclusions are referred in the rest of the article as ‘‘phase average’’. In Section 2, a description of the implementation of the different techniques is presented. The results are presented in Section 3; the results are discussed in Section 4. The conclusions are summarized in Section 5 of this article.

2. Methodology of the numerical experiments

2.1. Implementation of Mori–Tanaka and PGMT formulation

To compare the inclusion average stresses predictions by the Mori–Tanaka formulation and PGMT a series of VE was created. A second order orientation tensor ***‘‘a’’,*** was fed as an input to describe the orientation distribution of the inclusions [18] for all the calculations. Complete information about the orientations of inclusions is based on a fourth order orientation tensor. If the orientation is fixed or uniformly random the closure from second order orientation tensor ‘‘***a***’’ to the fourth order orientation tensor ***‘‘A’’*** is exact. However, if the orientations are neither uniformly random nor fixed, the estimation of the fourth order orientation tensor from the second order orientation tensor is not exact and some approximation is needed. In such cases, orthotropic closure method as described by Cintra and Tucker [19] was used for both the Mori–Tanaka and PGMT formulation.

Within the scope of this paper, we have considered a 2D distribution of orientations for reasons of simplicity. The orientation of inclusions is characterised by an angle $\boldsymbol{\varphi}$; this is defined as the orientation of the inclusion with respect to the global x-direction. Pseudo-grain discretization of such an VE consisting of inclusions with different orientations but with the same aspect ratio was done with the number of pseudo-grains equal to 30. In our case of 2D distribution of orientations each grain is characterised by an angle, phi φ. Each grain contains inclusions having an orientation angle between $\varphi \pm d\varphi$. A detailed description of the discretization of an VE to a number of pseudo-grains is described in [7]. PGMT calculations were performed using the software DIGIMAT [20]. For the Mori–Tanaka formulation a realization of 1000 inclusions was used in all the calculations.

2.2. Generation of finite element model

To perform the FE calculations, VE of the microstructure was built by using the random sequential adsorption algorithm [21]. It was not possible to have a quality mesh in ABAQUS [22] for ellipsoids with an aspect ratio higher than 5, so the aspect ratio chosen for the majority of the calculations was 3. Inclusions with a higher aspect ratio were modelled as a cylinder with semi-spherical ends. The placement of the inclusion centres was random in all cases. To ensure an acceptable mesh the minimum distance between two inclusions was 0.0035 times the diameter of the inclusion [23]. Periodic boundary conditions were applied to the three axis of the VE cube to approximate an infinite VE as closely as possible [24]. The periodic structure of the cuboidal cells is ensured by splitting the ellipsoids intersecting the edge of the cube into an