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

Atul Jain[1/2,*], Stepan V. Lomov[2], Yasmine Abdin[2], Ignace Verpoest[2], Wim Van Paepegem[3]

1. LMS International, N.V. Leuven, Interleuvenlaan 68, B-3001 Leuven, Belgium
2. Department of Metallurgy and Materials Engineering , KU Leuven, Belgium;
3. Department of Material Science and Engineering, Ghent University, Belgium

**Abstract:** For modelling damage in short fibre composites, both the predictions of the effective properties and the stresses in the individual inclusions and in the matrix are necessary. Mean field theorems are usually used to calculate the effective properties of composite materials, most common among them is 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 formulation and PGMT for 2D-orientation of inclusions. The average stresses inside inclusions and the matrix are compared to solutions of full-scale 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. However, 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. Mori-Tanaka must be used as the first choice homogenization scheme.

Key words: A-Short-Fiber Composites, C-Finite Element Analysis (FEA), C-Modelling, Mean-field homogenization

## 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 in the automotive industry to be used for semi-structural components. The predictions of various damage modes in short fiber composites components like fibre matrix debonding and fibre breakage requires the knowledge of both the effective properties of the composite and of the stresses and strains in the individual inclusions. The effective properties of composites are estimated, among other methods, using mean field homogenization schemes. Almost all mean field algorithms 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.

By using the Mori-Tanaka formulation one can calculate the effective stiffness of a composite by estimating first the strain concentration factor in the inclusions and then relating the effective stiffness of a composite to the strain concentration factor by the following relation

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

where, $C^{eff}$ is the effective stiffness of the composite, $C^m$, $C^\alpha$ are the stiffness matrix of the matrix and inclusion respectively, $c_\alpha$ is the volume fraction of individual inclusion, m is the total number of inclusions and $A^\alpha$ 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. Mori-Tanaka and self-consistent schemes were shown by Benveniste et al., [4] to 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 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 approach 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 as well and it is this extension from two-phase composites to multi-phase composites with differently shaped reinforcements, not the original Mori - Tanaka assumption that occasionally produces physically inadmissible results.

Pierard et al.[7] proposed a method to circumvent the mathematical problems of the Mori-Tanaka formulation. They discretized the representative volume element (RVE) to a number of “pseudo-grains”. A pseudo-grain is 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 RVE into several “pseudo-grains” was also implemented by Kaiser et al. [8]. We will call this “pseudo-grain” formulation of the Mori-Tanaka method in short the “PGMT” formulation.

A number of different works describing comparison of the predictions of the effective response of composite materials by various mean field theories with finite element simulations of microstructures can be found in literature, 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 fiber 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] focussed primarily on the comparison of predictions of effective mechanical properties of RVE. 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 is a function of the orientation of the inclusion. Duschlbauer et al. [17] compared predictions of stresses in individual inclusions by a modified Mori-Tanaka formulation and finite element results for a RVE with 2d-planar uniform random arrangement of carbon fibers in copper matrix. But apart from 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 predictions of stresses in individual inclusions by the Mori-Tanaka formulation and the PGMT formulation with finite element calculations. A number of different cases including aligned inclusions, non-aligned inclusions including both approximations of 2D-planar uniform random and also 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 are taken to be 3 while, the volume fraction of inclusions vary from 0.01 to 0.25. For all the cases considered, a uniaxial load case is applied and comparison is made for both the stresses in the applied load direction S11 as well as transverse loading direction S22. Average stresses in individual inclusions are referred in the rest of the article as “inclusion average”; while the average of stresses across all inclusions referred in the rest of the article as “phase average”. All the stresses are calculated in the global co-ordinate system of the orientation tensor. In section 2, a description of the implementation of the different techniques is presented. The results are presented in section 3, the results are discussion in section 4. The conclusions are summarized in section 5 of this article.

## 2. Methodology of the numerical experiments

To compare the inclusion average stresses predictions by the Mori-Tanaka formulation and PGMT a series of RVE were created. The volume fraction of the inclusions varied from 1% to 25%. For all the calculations, a second order orientation tensor ***“a”,*** was fed as an input to describe the orientation distribution of the inclusions [18]. 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 is exact. However for orientations which 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. In such a case, the orientation of inclusion is characterised by an angle **φ,** which is defined as the orientation of the inclusion with respect to the global x-direction. Pseudo-grain discretization of such an RVE, consisting of inclusions with different orientations but with same aspect ratio was done with the number of pseudo-grains equal to 30. Each pseudo-grain is characterized by orientation vector ***p***, and consists of a bi-phase composite containing inclusions whose orientation vector lies between ***p+dp***. In our case since of 2D distribution of orientation each grains is characterised by an angle, phi φ and contains all inclusions having orientation between angle φ±dφ. A detailed description of the discretization of an RVE 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.

## 2.1 Generation of finite element model

For the finite element calculations, a volume element (VE) of the microstructure was built by using the random sequential adsorption algorithm[21]. For building the finite element model, meshing ellipsoids in the finite element solver ABAQUS [22] proved to be challenging for inclusions with aspect ratio higher than 5. Keeping this in mind, 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 all the three axis of the VE cube to approximate an infinite VE as close as possible. Periodic structure of the cuboidal cells is ensured by splitting the ellipsoids intersecting the edge of cube into appropriate number of parts which is then copied to the opposite face of the cube. Three faces of the cube are meshed and then copied to the corresponding opposite face to ensure identical meshes on opposite faces. Periodic boundary conditions are applied to the cubic cell by applying the following equations:

$$\boldsymbol{u}(x, y, 0) - \boldsymbol{u}_z = \boldsymbol{u}(x, y, L)$$

$$\boldsymbol{u}(x,0,z) - \boldsymbol{u}_y = \boldsymbol{u}(x,L,z) \qquad (2)$$

$$(0,y,z) - \boldsymbol{u}_x = \boldsymbol{u}(\alpha L,y,z)$$

Where, $\boldsymbol{u}$ is the displacement vector in the different faces of the cube and $\boldsymbol{u}_x$, $\boldsymbol{u}_y$, $\boldsymbol{u}_z$ depend on the particular loading applied to the cubic cell. Uniaxial strain $\varepsilon_x$ is applied by $\boldsymbol{u}_x = (\varepsilon_x \alpha L,0,0)$, $\boldsymbol{u}_y = (0, u_y, 0)$ and $\boldsymbol{u}_z = (0,0, u_z)$. $u_y$ and $u_z$ is then computed from the conditions.

$\int_\Omega T_y \, d\Omega = 0$ on $y = L$ and $\int_\Omega T_z \, d\Omega = 0$ on $z = L$. Where $T_y$ and $T_z$ are the normal tractions acting on the prism faces contained in the transverse planes $y = L$ and $z = L$. Similar boundary conditions can be applied for different loading directions as well. The ABAQUS solver was used to solve the finite element problem with C3D10M elements – a 10 node tetrahedron element (figure 1a, 1b, 1c), this was as prescribed by software DIGIMAT.

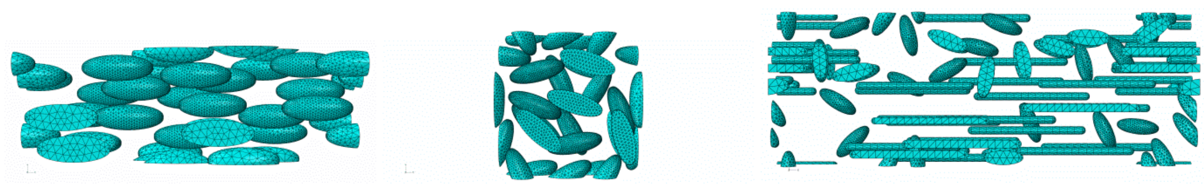


**Figure 1** Periodic cuboid showing Finite element Volume element(VE) Notice that the structure is periodic and inclusions intersecting a face of cube also appear on the opposite face.
**Figure 1a** VE containing 30 inclusions aligned in same direction, volume fraction of inclusions is 0.161 and aspect ratio is 3. **Figure 1b** VE containing 30 inclusions having an approximate uniform random distribution of inclusions with orientation tensor (a11=0.52, a22=0.48) and a volume fraction of 0.25. **Figure 1c** VE having inclusions with aspect ratios 3 and 15; the orientation of the inclusion with lower aspect ratio is uniformly random, while longer inclusions are aligned in one direction. The volume fraction of the both the phases are 0.05.

2.2 Description of models considered

The calculations performed can be grouped into three categories. A first set of models studied had inclusions with aspect ratio 3 and volume fraction 0.161 (equivalent to mass fraction of 30%, which is a typical value for injection moulded composites) were fully aligned to each other. For this case, two RVE are considered the first one had all the inclusions aligned in the same direction with value of orientation angle $\varphi=0$, whereas the second model has all inclusions with value of orientation angle *φ=90*. This set of calculations was performed to compare the predictions of the Mori-Tanaka formulation with the FE results. PGMT for such configurations is equivalent to Mori-Tanaka formulation, since such an RVE which is already a biphase composite, pseudo-grain discretization leads to creation of a single pseudo-grain.

A second set of models was built with approximate 2D-planar uniformly random orientations. The different volume fractions considered were 0.01, 0.1 and 0.25%. A third set of calculations were aimed at comparing the predictions of the Mori-Tanaka and the PGMT formulation when the assumptions of mean strain and image strain were said to be too simplistic [24]. First a model with non-uniform 2D-planar orientation is considered. Inclusions had an aspect ratio of 3, while the orientation distribution for this case was taken to be a11= 0.65, a22=0.35. Finally a comparison was made for the case of mixed aspect and mixed orientations, the model consisted of inclusions having aspect ratio 3 and 15. The inclusions with aspect ratio 15 were modelled as a sphero-cylinder while the inclusions with aspect ratio 3 were modelled as ellipsoids. The orientation of the inclusion with lower aspect ratio is an approximation of 2D-planar uniform random, while longer inclusions are aligned in one direction. This particular configuration was chosen to create a RVE so as to test the validity of the assumptions of the Mori-Tanaka formulation even in cases when there are inclusions with different aspect ratios as well as completely different orientation tensor for inclusion of each aspect ratio. A summary of the different volume elements considered are presented in table 1.

Table 1: A summary of the different cases considered

| Sl. No. | Description of inclusions in different models considered | Volume fraction of inclusion |
|---|---|---|
| 1 | Fully aligned inclusions with an aspect ratio 3, orientation angle, φ=0 | 0.161 |
| 2 | Fully aligned inclusions with an aspect ratio 3, orientation angle, φ=90 | 0.161 |
| 3 | Inclusions with aspect ratio 3 having orientation distribution close to uniform random; a11= 0.54, a22=0.46 | 0.01 |
| 4 | Inclusions with aspect ratio 3 having orientation distribution close to uniform | 0.1 |

| | | |
|---|---|---|
| | random; a11=0.51, a22=0.49 | |
| 5 | Inclusions with aspect ratio 3 having orientation distribution close to uniform random; a11=0.52, a22=0.48 | 0.25 |
| 6 | Inclusions having aspect ratios 3 and 15; the orientation of the inclusion with lower aspect ratio is uniformly random, while longer inclusions are aligned in one direction | 0.05 of each phase |

Finally the effect of pseudo-grain discretization on the stress predictions of the matrix region was compared.

### 2.3 Size of Finite element model and checking for transverse isotropy

Under periodic boundary conditions, the number of inclusions required to completely characterize an VE depends on the volume fraction of the inclusion phase. There are no theoritical estimations for minimum size of VE having anisotropic inclusions[25]. In such cases the accuracy of the numerical simulations is usually established by comparing the scatter in the effective response for different dispersions of reinforcements; this technique was used by Seguardo et al.[26] and Pierard et al.[27]. For a composite having inclusions of aspect ratio 3 and a volume fraction of 0.25 Pierard et al.[27] concluded that 30 inclusions was enough to limit the standard deviation in predictions of effective response to less than 1% even in the non-linear regime, 30 was thus seen as sufficient number of inclusions to form a VE.

For our study, we decided to confirm this calculations for the same configurations as considered by Pierard et al. [27], but the constituent fiber and matrix properties are different. This particular configuration of inclusions with aspect ratio 3 and volume fraction of 0.25 is considered because in the study presented in this paper, the highest volume fraction considered is also 0.25. Multiple dispersions of volume elements with 10, 20 and 30 inclusions each subjected to an applied uniaxial strain of 1%. Like Pierard et al. [27] we noticed that mean of averages stresses in the volume element for different realizations for 10, 20, 30 inclusions were practically the same and equal to the Mori-Tanaka predictions of 60.2 MPa. We then assumed that the size of an VE would be sufficient if for an applied strain, the average stresses of the volume element in the different realizations didn't vary by more than 5% from each other. We found that for 20 inclusions, the difference between the maximum and minimum value of average stresses in the volume element was less than the desired 5%, the maximum and minimum values of average stresses in the different realizations of the volume element was 58.6 and 62 MPa respectively. We however used 30 inclusions for most calculations.

For the case of 2D-planar uniform random orientation described in section 2.2, the required orientation distribution tensor is $a_{11}=a_{22}=0.5$. A Finite element VE with 30 inclusions having aspect ratio 3 was created with a uniform random orientation of inclusions. Upon recalculation of the orientation tensor of the concrete VE based on the 30 inclusions, it was seen that there were some deviations from the ideal 2-D planar uniform random orientation. It was not possible to get strictly uniform random orientation for an VE with only 30 inclusions. A realization of volume element was considered to be a reasonable approximation of 2D-uniform random if the difference in effective response for axial and transverse loading is less than was within 5% of each other. This condition of 5% deviation in the effective response of volume element is the same condition as was choosen for estimating the minimum size of the volume element. The input orientation tensor for the mean field homogenization (both Mori-Tanaka and PGMT formulation) was the value of the orientation tensor recalculated from the orientations of the 30 inclusions in the FE model.

The phase average stresses were calculated as a volume weighted average of the stresses in the elements forming the inclusion phase. For all the calculations, the inclusion phase was isotropic glass fibre and matrix was polyamide with an Young's modulus of 72 GPa and 3 GPa respectively, while the Poisson's ratio was 0.22 and 0.37 respectively.

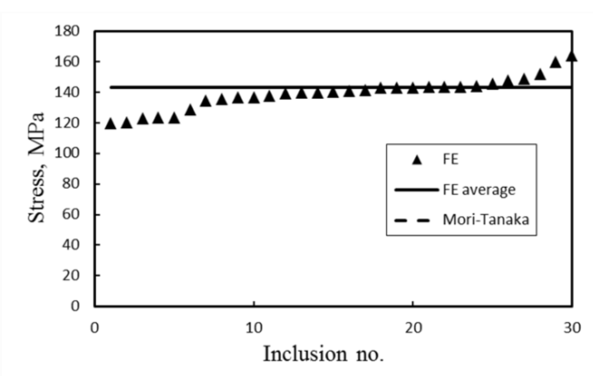
## 3. Results

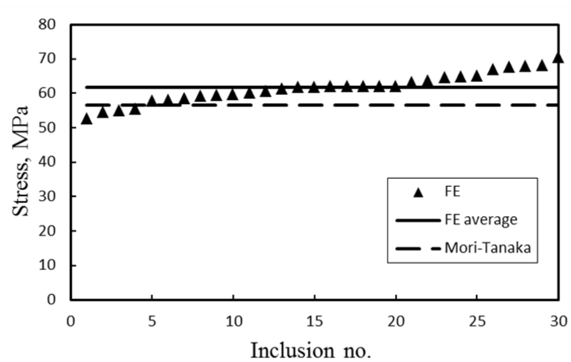
A comparison of predictions for both inclusion average and phase average for a wide range of cases is presented in this section.

### 3.1) Mori-Tanaka formulation for fully aligned cases

For all model containing inclusions with orientation, $\varphi$=0, the predictions of phase average stress in the inclusions in the axial directions (S11) by the Mori-Tanaka formulation was 143.3 MPa compared to 143.2 MPa (figure 2a.) in the FE model. While for the case where all inclusions had value of orientation angle, *$\varphi$=90,* the Mori-Tanaka formulation phase average predictions of stresses in axial direction (S11) was 56.6 MPa, which was higher than the predictions of FE which was 61.6 MPa (figure 2b). In both the cases, the Mori-Tanaka formulation slightly underestimated the phase average stresses when compared to the values predicted by the FE model.

There is also some scatter in the stress levels of the individual inclusions in the FE model, particularly in the transverse direction (figure 2c, figure 2d); this could be due to the fact that the immediate neighbourhood of the inclusions is different for the inclusions. For a confidence interval of 95%, the range was calculated to be 3.75MPa and 1.52 MPa respectively for 1a and 1b respectively.



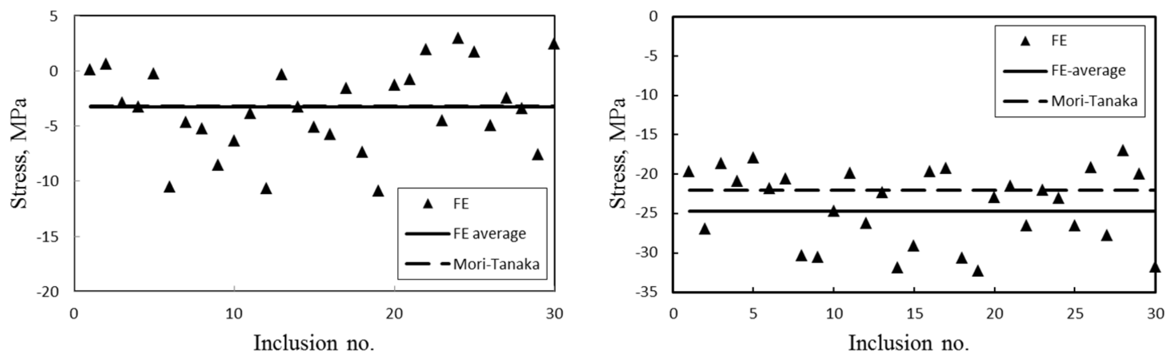



**Figure** 2 Inclusion average and phase average stresses for an RVE with fully aligned inclusions, with aspect ratio 3 and *vf* = 0.164 for an applied strain of 1%, **Figure 2a** S11 for inclusions have ϕ = 0, **Figure 2b** inclusions have ϕ = 90, **Figure 2c** S22 for inclusions have ϕ = 0, **Figure 2d** S22 for inclusions have ϕ = 90.

3.2) Mori-Tanaka formulation and PGMT for random orientation of inclusions

The first step in this set of calculations is to ascertain whether the orientation distribution of the finite element model was a sufficient approximation of uniform random. First for the case when the volume fraction of inclusions is 0.01, for uniaxial loading of 1% strain, the orientation tensor recalculated from the discrete finite element volume element was (a11=0.54, a22=0.46). When subjected to loading in the axial direction, the average stresses in the axial direction was calculated to be 30.4MPa, while for the transverse loading the average stresses in the volume element was 30.1 MPa. Similarly for the case when the volume fraction of the inclusion was 0.1, the orientation tensor recalculated from the discrete finite element volume element was (a11=0.51, a22=0.49). Average stresses for axial and transverse loading was 34.6MPa and 34.5Mpa repectively. In the final case when the volume fraction of the inclusions was 0.25 the orientation tensor recalculated from the discrete finite element VE was (a11=0.52, a22=0.48). Average stresses for axial and transverse loading was 55.7MPa and 54.4MPa respectively. Thus in all the three cases we were able to ascertain that our finite element models were reasonable approximations of the ideal 2d-uniform random case. The inclusion average stresses, S11 was found by all the three methods to follow a quasi-sinusoidal trend as a function of the orientation of the inclusion. The inclusions with orientations closer to 0° with respect to the loading axis were stressed higher than the ones with higher orientation angles. However the peak in the curve of PGMT was much flatter than in the predictions by both Mori-Tanaka and full finite element calculations. The predictions by the PGMT were off significantly in all the cases. The predictions by both the Mori-Tanaka formulation and FE were however in excellent agreement with each other for both the axial (figures 3a, 3b, 3c) and transverse stresses (figures 4a, 4b, 4c) for all the three volume fractions considered. The scatter in the FE results was found to be increasing with increase of the volume fraction.

The phase average stress in the inclusion phase was quite close to each other by all the MT, PGMT as well as full finite element calculations. For the RVE with volume fraction of 0.01 the predictions of phase average stresses were 78.9, 78.9 and 78.2 MPa for the Mori-Tanaka formulation, PGMT and FE calculations. Similarly the values of phase average stresses for the three methods was 83.7, 83.8 and 87.1 MPa respectively when the volume fraction was 0.1 and 101, 100.6 and 104.2 MPa when the volume fraction was 0.25. The average stiffness of the composite is a direct function of the phase average stress (and strain). Because both methods give similar values of the phase average stress; both the methods, namely MT and PGMT can be expected to give similar predictions of the effective stiffness.

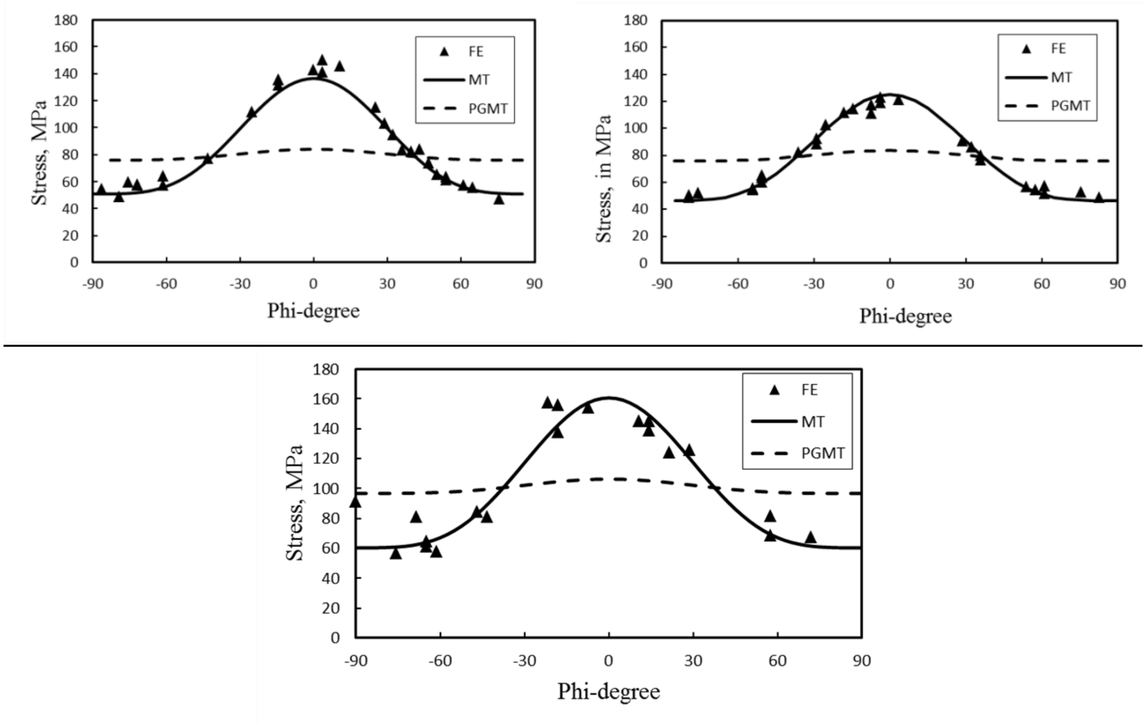



**Figure 3** Inclusion average stresses in the global loading direction, S11 for random orientation of inclusions, applied load is 1% strain , **figure 3a** *vf* = 0.1, with orientation tensor (a11=0.51, a22=0.49); **figure 3b** *vf* = 0.01, with orientation tensor (a11=0.54, a22=0.46) **figure 3c** *vf* = 0.25**,** with orientation tensor (a11=0.52, a22=0.48).

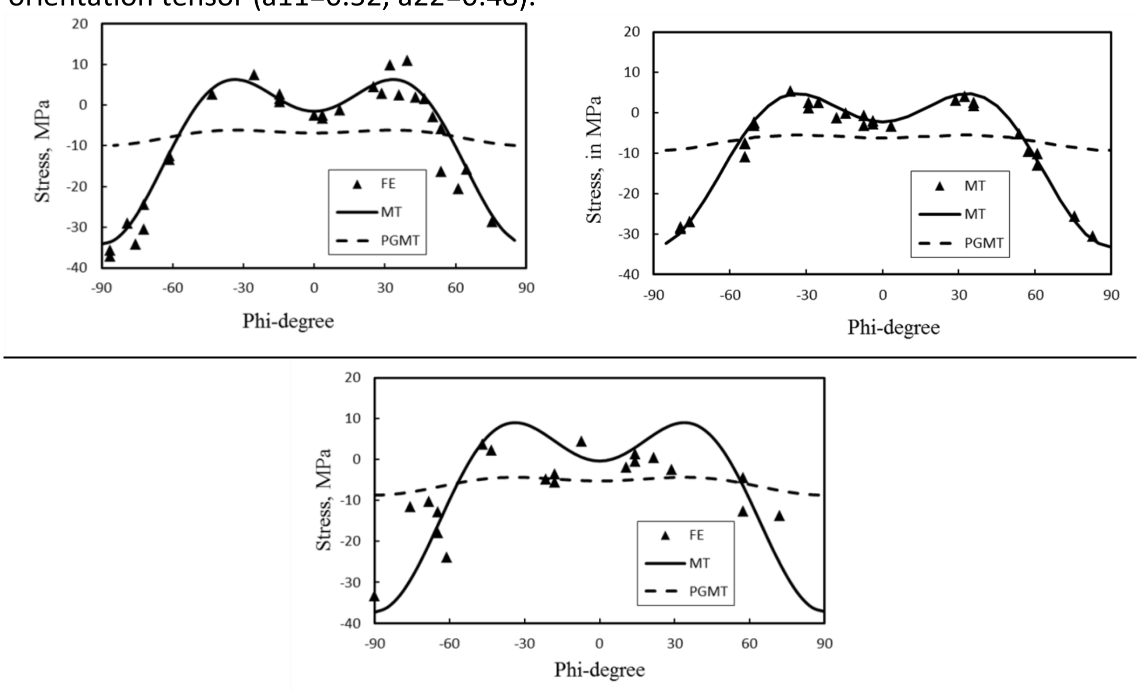



**Figure 4** Inclusion average stresses transverse to the global loading direction, S22 for random orientation of inclusions, applied load is 1% strain. **figure 4a** *vf* = 0.1, with orientation tensor

(a11=0.51, a22=0.49); **figure 4b** *vf* = 0.01, with orientation tensor (a11=0.54, a22=0.46) **figure 4c** *vf* = 0.25, with orientation tensor (a11=0.52, a22=0.48).

3.3) Mori-Tanaka formulation and PGMT for non-uniform distribution of inclusions

In all the cases studied in section 3.2 the orientation of inclusions was close to uniform random. The assumption of uniform mean stress was described as reasonable for bi-phase composite and composites with ideal uniform random orientation of inclusions [4, 6, 24]. The results shown in previous section are in good agreement with this conclusion. A FE model was now created where the orientation distribution was not the ideal 2-D planar uniform random, which was analysed in the section 3.2. The orientation tensor recalculated from the discrete finite element volume element was ($a_{11}$=0.65, $a_{22}$=0.35). The effective stress response to axial and transverse loading for this model was 54.7 and 45.5 respectively, thus there is a 16.67% difference which is more allowed 5% deviation for 2D-planar uniform random case. Like was seen in the previous calculations, the Mori-Tanaka formulation was in excellent agreement with the FE results, while PGMT once again led to poor correlation. (Figure 5a, 5b). The mean-strain assumption of the Mori-Tanaka formulation might be valid even for a statistical distribution of orientations and PGMT leads to no obvious advantages in terms of predictions of inclusion average stresses. The predictions of average stress in the inclusion phase were once again very close to each other for all the three methods of analysis. The predictions for MT, PGMT and full FE calculations were 100.7, 101.1 and 103.7 MPa respectively.

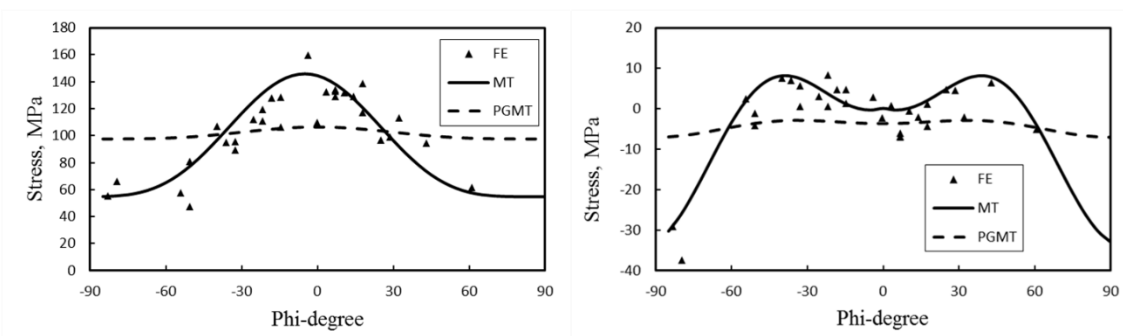
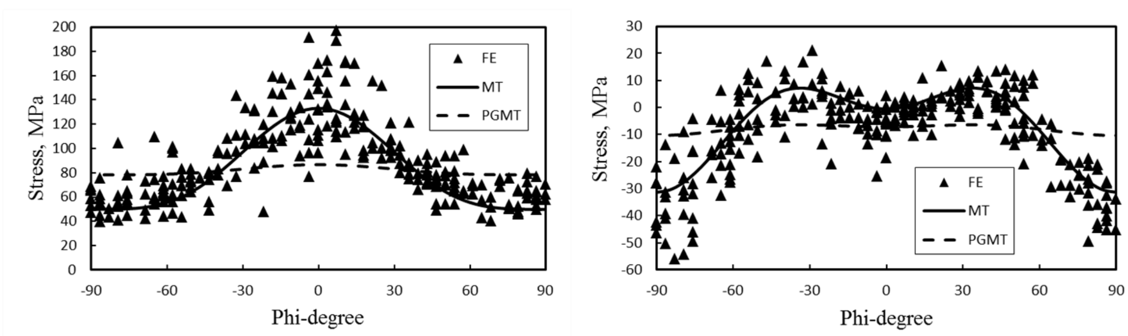


**Figure 5** Aspect ratio of inclusions = 3, vf = 0.164 and orientation tensor (a11=0.65, a22=0.35). Applied load is 1% strain.**Figure 5a** Inclusion average stresses in loading direction. **Figure 5b** Inclusion average stresses in transverse to loading direction.

For the case with distributed length of inclusions. The inclusion average of stress predicted by FE showed a significant scatter. PGMT once again gave a poor prediction. To better understand the scatter and validity of the predictions of the Mori-Tanaka formulation, a number of different realizations of VEs with the similar configurations (for the inclusions with aspect ratio 3, the orientation tensor components $a_{11}$ and $a_{22}$ varied in the range of 0.48 to 0.52) were created. It was seen that the FE predictions of the inclusion average stresses formed a scatter cloud to the predictions of the MT (figure 6a, 6b).

Each realization of the VE has a unique combination of orientations of inclusions. On creating about 20 different realizations of the volume element, we were able to get at least 7 different inclusions for most orientation of inclusion, φ. The inclusion average stresses for every orientation were averaged. Predictions of average inclusion stress by the Mori-Tanaka formulation were found to be in excellent agreement with the mean value of the inclusion average stresses calculated from different FE realizations (figure 6c, 6d). The confidence interval for significance level alpha = 0.05 is shown in the figure and is in the range of 10-15% of the mean value for most inclusions.



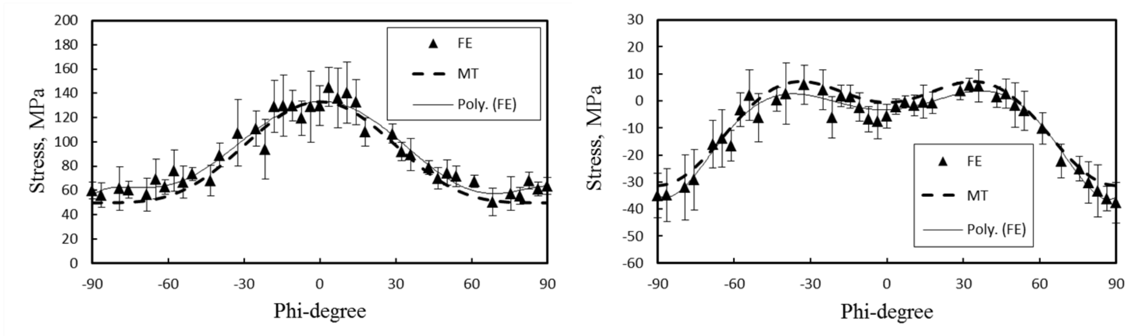


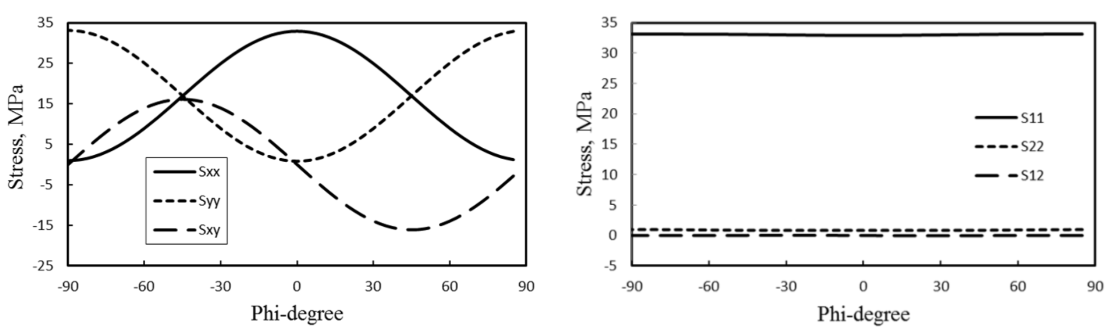

**Figure 6** The scatter of average stresses in inclusions with respect to orientation for inclusions with aspect ratio 3. RVE consisted of randomly oriented inclusions with aspect ratio 3 and aligned inclusions with aspect ratio 15. **Figure 6a V**ariation of S11 **Figure 6b** Variation of S22. **Figure 6c** Polynomial curve fit of mean of inclusion average stresses of FE, also displaying confidence interval of α=0.05 of stresses for S11 **Figure 6d** Polynomial curve fit of mean of inclusion average stresses of FE, also displaying confidence interval of α=0.05 of stresses for S22.

The stresses in the fully aligned inclusions having aspect ratio of 15 were predicted higher by both the mean field schemes when compared to the FE calculations. The average stresses in the individual inclusions varied from 321 MPa to 543 MPa with the average being 420 MPa in the FE calculation and 489 MPa and 475 MPa for Mori-Tanaka and PGMT respectively. The phase average stresses were predicted to be 259.8, 278, 285.9 MPa for FE, Mori-Tanaka formulation and PGMT respectively. The Mori-Tanaka formulation and PGMT predict marginally higher values of phase average stresses when compared with the FE calculations, but are once again close to each other.

### 3.4) <u>Effect of pseudo-grain discretization on the stresses in the matrix</u>

The matrix is treated differently in the three methods namely, the Mori-Tanaka formulation, the PGMT and the FE analysis. In the Mori-Tanaka formulation, the matrix is treated as one continuous medium while the matrix is discretized into a number of pseudo-grains in the PGMT formulation. In FE calculations, the matrix is broken into numerous elements and the stresses are calculated for each element. A direct comparison of the three methods is thus not possible.

In the PGMT formulation the matrix stresses in the different grains are calculated in different inclusion local-axis systems. For random orientation of inclusions with $a_{11}$=0.65, $a_{22}$=0.35, and aspect ratio 3 and a volume fraction of 0.164, the values of the matrix stresses in the different grains were different in their corresponding local systems. However, when these stresses were transformed to the global axis the difference was less than 1 per cent for all the above cases and also in excellent agreement with the Mori-Tanaka formulation. The variation of matrix stresses in different pseudo-grains is as shown in figure 7a and 7b. Thus, there is no observable difference in the values of the strains (and stresses) in the matrix with or without pseudo-grain discretization. The predictions of the finite element model showed a huge range of stresses in the matrix elements. A histogram with the variation of stresses in elements predicted by FE is shown in figure 7c. Neither the Mori-Tanaka formulation nor the PGMT managed to capture the huge variation of stresses in the matrix region. This is expected as both the Mori-Tanaka and the PGMT formulation give the value of matrix stresses in an average sense, nullifying completely the effect of stress concentration in the matrix region around the inclusions.



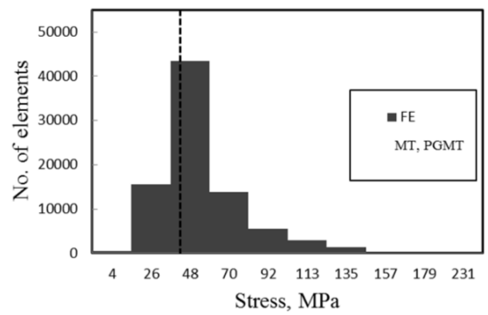



**Figure 7a** Stresses in matrices in local grain axis for PGMT formulation. **Figure 7b** Stresses in matrix in global axis for PGMT formulation. **Figure 7c** Histogram showing the variation of global stresses in individual matrix elements in the FE calculations, with predictions of the Mori-Tanaka and PGMT formulation**.**

## 4. Discussion:

As discussed above, the Mori-Tanaka formulation predicted correctly the inclusion average stresses whereas the pseudo-grain discretization led to incorrect prediction of the inclusion average stresses. After pseudo-grain discretization the individual inclusions are discretized in a field of inclusions having same orientation and aspect ratio to itself is therefore influenced by only inclusions which have orientation and aspect ratio. PGMT formulation seperates inclusions at a scale which it shouldn't, this leads to loss of some interactions between the inclusions and also introduces spurious interactions between inclusions having the same orientation and aspect ratio.

Both the Mori-Tanaka and PGMT formulations predicted similar values of the phase average stress. For the case of the Mori-Tanaka formulation the stresses (and strains) in the individual inclusions are averaged to estimate the strain concentration factor which is then used to calculate the effective stiffness. However, in PGMT, the effective stiffness of the individual grains is first estimated by the Mori-Tanaka formulation and then the effective stiffness of the composite is calculated as a volume weighted average of the stiffness of the individual grains. In a composite material having isotropic inclusions and matrix showing linear behaviour, the pseudo-grain discretization is equivalent to redistributing the image strain unevenly among the inclusions. In such cases the predictions of phase average stresses of PGMT should be in good agreement with the predictions of Mori-Tanaka. This is also what was observed in our calculations.

## 5. Conclusions

Comparisons for stress predictions by the Mori-Tanaka formulation and PGMT for individual inclusions were performed for a wide range of inclusion configurations, each having atmost a 2D-orientation of inclusions. In all the cases the Mori-Tanaka formulation proved to give good correlation with the finite element calculations. Pseudo-grain discretization however failed to give good estimates of the stress level in the individual inclusions while predicting correctly the phase average stresses. The assumption of the mean strain in the Mori-Tanaka formulation seems to be a reasonable estimate, even in cases when there was statistical distribution of orientation and length in inclusions. For the matrix phase, no significant differences were reported in the prediction of stress levels by full Mori-Tanaka formulation and by Mori-Tanaka formulation after pseudo-grain discretization.

The scatter of deviation of the FE results for individual inclusions from the average trends predicted by the Mori-Tanaka formulation increases with increase in volume fraction of inclusion and also quite significantly when there is a length distribution. In such cases, the Mori-Tanaka formulation can only predict the general trend of stresses in inclusions with respect to orientations. It can be concluded that Mori-Tanaka formulation is a better approximation of reality and should be used as the standard ("first choice") mean field homogenization method, particularly if the stresses in individual inclusions are important for further analysis.

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