# Mori-Tanaka calculations of strains in ellipsoidal inclusions with multiple orientations.

## Comments on the papers: Naili, G. et al Comp Sci Tech, 187: 107942, 2020 (https://doi.org/10.1016/j.compscitech.2019.107942) and Jain, A. et al, Comp Sci Tech, 87: 86-93, 2013 (https://doi.org/10.1016/j.compscitech.2013.08.009)

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Mean field homogenization (MFH) is a widely accepted approach for the prediction of effective properties of composites. Calculating the local stresses in individual inclusions is a more challenging exercise, particularly since the MFH methods are based on average strain fields. Jain et al. [1] and recently Naili et al. [2] have reported contradictory results for a particular homogenization scheme. This note indicates and rectifies an error in [1], and eliminates the mentioned contradiction.

Naili et al. [2] compared the predictions of strains in inclusions by two methods viz. FE-MT and FE-Voigt for a representative volume element (RVE) containing 2D ellipsoidal inclusions. In these schemes, multiphase composites were homogenized by first homogenizing pseudo-grains consisting of fibers having the same orientation using full field Finite Element (FE) simulations. The second step of the homogenization was subsequently performed using the Mori-Tanaka (MT) formulation (designated as "FE-MT") and the Voigt approximations ("FE-Voigt") respectively. FE homogenization was chosen as the first step of homogenization to ensure that the comparison is "unbiased". It is known that for uni-directional composites, the MT formulation and FE yield identical results for effective stiffness as well as the strains in the inclusions. Thus, the first step of homogenization could have been MT formulation with no or little change in the results. Further, Naili et al. show that MT-MT (MT homogenization in both steps) is equivalent to the full analytic MT formulation.

Naili et al. have shown that the strain predictions for individual inclusions by the two methods (FE-MT and FE-Voigt) are very close to each other. As noted by Naili et al., these results are in direct contradiction with results published by the authors of the present comment [1], where the strain/stress predictions by the MT and the MT-Voigt schemes were significantly different.

In [1] the MT-Voigt calculations were not done explicitly, but were the results of an output from software DIGIMAT [3], which is based on the MT-Voigt scheme. To ascertain the differences in result, the results in the paper by Jain et al. [1] have been recalculated using analytic formulae, prescribed by Naili et al., with one difference: Naili et al. used full FE for the homogenization of the pseudo-grains, while the MT method has been used here. As noted above, this difference should not affect the results significantly. The RVE considered for comparison consisted of inclusions with aspect ratio equal to 3, having Young's modulus, E = 72 GPa and Poisson's ratio equal to 0.22 while the corresponding properties of the matrix were 3 GPa and 0.37 respectively. The orientation distribution of the inclusions is approximately uniformly random in one plane (the second order orientation tensor has components $a_{11}$=0.52 and $a_{22}$=0.48; as opposed to $a_{11}$=0.50 and $a_{22}$=0.50 for uniform random orientation) and the volume fraction of the inclusions is 0.25.

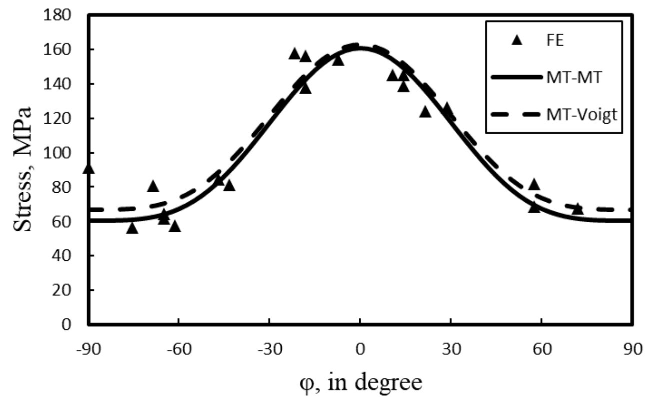


**Figure 1** *Inclusion average stresses of VE with inclusions with aspect ratio = 3, $v_f$=0.25 and orientation tensor (a11=0.52, a22=0.48). Applied load is 1% strain. (a) Stress component, S11 (FE data extracted from Jain et al. [3]). $\varphi$ is the Eulerian angle*

It is confirmed that MT-MT and MT-Voigt are in a very good agreement, also in a good agreement with FE (**Figure 1**). This is in correspondence with the conclusions in Naili et al, which are based on similar calculations with 2D geometry of the ellipsoidal inclusions.

It is thus established that the MT-Voigt data reported by the present authors in [1] is erroneous. This error is most likely caused by an unidentified error in software DIGIMAT or in accessing the DIGIMAT data during the calculation of the stress in individual inclusions. The conclusions of Naili et al. stating that the strain predictions by MT-MT and MT-Voigt schemes for random RVE are similar, are confirmed to be correct, and our conclusions on differences between the two schemes are wrong. The correctness of the conclusions of [2], based on the 2D-random case, is additionally proved by extending the analysis to a 3D-random case.

Naili et al. derive the expressions for the strain in the inclusions using the two schemes, viz. FE-MT and FE-Voigt based on the results of the FE simulation in the first step of homogenization. Mathematically, the average strain in an inclusion, $\langle\varepsilon\rangle_{w^f_{\vec{p}}}$ (we follow the notations of [2]) according to the FE-MT scheme is given in equation 1

$$\langle\varepsilon\rangle_{w^f_{\vec{p}}} = B^f_{\vec{p}}\colon\left(v_m + (1 - v_m) < B^f_{\vec{p}} > \varphi\right)^{-1}\colon\langle\varepsilon\rangle_w \quad (1)$$

Where, $B^f_{\vec{p}}$ is the partial strain concentration tensor, $< >\varphi$ indicates orientation averaging and $v_m$ is the volume fraction of the matrix phase. According to FE-Voigt, $\langle\varepsilon\rangle_{w^f_{\vec{p}}}$ depends on the strain concentration tensor, $A^f_{\vec{p}}$ (equation 2)

$$\langle\varepsilon\rangle_{w^f_{\vec{p}}} = A^f_{\vec{p}}\colon\langle\varepsilon\rangle_w \quad (2)$$

It must be noted that both the strain concentration tensor and partial strain concentration tensor are derived from the homogenization of the pseudo-grain and will be in the coordinate axis system coinciding with the axis system of the inclusion; coordinate transformation is needed for deriving the strains in inclusions with varying orientations. The stress in an inclusion is the product of the stiffness of the inclusion and the strain calculated by equation 1 or 2 depending on the choice of the scheme.

Equations 1 and 2 are fundamentally different in the sense that the equation 1 (for FE-MT) involves orientation averaging of the partial strain concentration tensor over the entire RVE while according to the equation 2 (for FE-Voigt), the strain in a certain inclusion is just a function of the strain concentration tensor derived from the homogenization of the pseudo-grain and the local orientation of the inclusion with no influence of the orientation distribution of the inclusion in the representative volume element (RVE). In other words, according to the FE-MT formulation, fibers with different orientations influence the strain in a particular inclusion, while the FE-Voigt does not account for this interaction. The 2D case investigated in [1] and the 3D case investigated here show a small difference between the two cases, in spite of this difference. However, it may be that there exist scenarios when the differences between MT-MT (1) and MT-Voigt (2) formulations could be significant.

To conclude, it is confirmed that the FE-MT and FE-Voigt schemes give very similar predictions for stresses in individual inclusions for composites with random orientation distribution of inclusions. Naili et al. confirm the match for a RVE with 2D random inclusions, while the match for 3D ellipsoid inclusions is confirmed here. The MT based methods (both analytic MT and MT-Voigt) are confirmed to give reasonable predictions both for homogenized properties and the stresses/strains in inclusions. However, confirming that the similar strain/stress predictions by both MT-MT and MT-Voigt will always be similar for RVE with varying length, modulus or non-random orientation distribution of inclusions requires a more thorough study given the very different expressions for strain in inclusions by the two schemes.

References:

[1] Jain A, Lomov SV, Abdin Y, Verpoest I, Van Paepegem W. Pseudo-grain discretization and full Mori Tanaka formulation for random heterogeneous media: Predictive abilities for stresses in individual inclusions and the matrix. Compos Sci Technol 2013;87:86–93. doi:10.1016/j.compscitech.2013.08.009.

[2] Naili C, Doghri I, Kanit T, Sukiman MS, Aissa-Berraies A, Imad A. Short fiber reinforced composites: Unbiased full-field evaluation of various homogenization methods in elasticity. Compos Sci Technol 2020;187:107942. doi:https://doi.org/10.1016/j.compscitech.2019.107942.

[3] www.e-Xstream.com, editor. DIGIMAT. Multi-Scale Model Platf 2019. doi:www.e-Xstream.com.