ON ADEQUACY OF THE HASHIN-SHTRIKMAN VARIATIONAL PRINCIPLES APPLIED TO POLYMER MATRIX BASED RANDOM FIBROUS COMPOSITES

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Summary. The paper offers a critical comparison between the finite element (FE) simulations exploiting the unit cell model and the two-point averaging scheme derived from the application of the Hashin-Shtrikman variational principles to nonlinear viscoelastic random fibrous composites. The presented results suggest that in attempt to reduce the computational cost, e.g., with the help of two-point averaging scheme, a caution must be exercised particularly in applications that include localization of inelastic deformation in one of the phases. Owing to its inherited stiffness the simplified two-point averaging schemes often fail in delivering realistic macroscopic response easily provided by the finite element simulations, however, at the expense of computational cost. Nevertheless, if the detailed local response is not of the main interest certain modifications to the standard format of the two-point averaging schemes can be introduced to arrive at the macroscopic response sufficiently close to the predictions derived from the finite element simulations on small statistically equivalent periodic unit cells.

1 INTRODUCTION

Proper description of the time-dependent behavior of textile polymer matrix-based composites is one of the most important characteristics in arriving at successful prediction of the mechanical response of these material systems. Owing to their geometrical complexity the macroscopic analysis of large structural elements usually calls for multi-scale or multi-level homogenization approach. The computational complexity increases with possibly random distribution of reinforcements on both micro and meso-scales. Here, we limit our attention to fibrous composites with random distribution of fibers within the transverse plane referred to as micro-scale (e.g., level of fibers within a tow of wound or textile composites, Fig. 1(a)).

2 MESOSCOPIC RESPONSE OF FIBER BUNDLE

Two possible approaches that account for random distribution of fibers are available. Both draw upon the existence of two-point probability function¹ S_{rs} . In the first approach



Figure 1: a) Micrograph of random fibrous composite, b) Binary image, c) 5-fiber SEPUC

based on finite element simulations the two-point probability function is used to generate statistically equivalent periodic unit cells (SEPUC) with a small number of particles such that both the SEPUC and the actual material system are described by the same statistics up to second order statistical moments. This is accomplished by minimizing the function

$$F(\{\mathsf{x}\}^{N}, H_{1}, H_{2}) = \sum_{i=1}^{N_{m}} \left(S_{0}(r_{i}, s_{i}) - S(r_{i}, s_{i}) \right)^{2},$$
(1)

where vector $\{x\}$ stores the positions of centers of individual particles (fibers) and H_1, H_2 are dimensions of the SEPUC. Example appears in Fig. 1(c). Once the SEPUC is derived standard homogenization procedure of periodic fields is introduced in the framework of the Hill lemma²

$$\langle \delta \{ \varepsilon \}^{\mathsf{T}} \{ \sigma \} \rangle = \delta \{ \mathsf{E} \}^{\mathsf{T}} \{ \Sigma \}, \tag{2}$$

to arrive at the distribution of local stress $\{\sigma\}$ and strain $\{\varepsilon\}$ fields in the composite loaded either by macroscopically uniform strains $\{\mathsf{E}\}$ or stresses $\{\Sigma\}$.

The second approach employs the well known Hashin-Shtrikman variational principle (HSVP) that allows a direct implementation of the two-point probability function in the formulation that leads to a set of algebraic equations for unknown polarization stresses $\{\tau_s\}$ in a given phase s in the form

$$\sum_{s=1}^{n} \left(\delta_{rs} ([\mathsf{L}_{\mathsf{r}}] - [\mathsf{L}_{\mathsf{0}}])^{-1} c_{r} - [\mathsf{A}_{\mathsf{rs}}] \right) \{ \tau_{\mathsf{s}} \} = \{\mathsf{E}\} c_{r} + ([\mathsf{L}_{\mathsf{r}}] - [\mathsf{L}_{\mathsf{0}}])^{-1} \{ \lambda_{\mathsf{r}} \} c_{r}, \tag{3}$$

$$[\mathbf{A}_{rs}] = \int_{\Omega} \left[\epsilon_{\mathbf{0}}^{*} \right] (\mathbf{x} - \mathbf{x}') \left(S_{rs}(\mathbf{x} - \mathbf{x}') - c_{r}c_{s} \right) \mathrm{d}\mathbf{x}'.$$
(4)

Binary images Fig. 1(b) of real micrographs Fig. 1(a) are usually used to derive the two-point probability function S_{rs} that appears in the definition of certain microstructure dependent matrices $[A_{rs}]$ in Eq. (4). In Eqs. (3)-(4) $[L_r]$, $\{\lambda_r\}$, c_r represent the phase elastic stiffness matrix, the eigenstrain vector that stores inelastic effects, and volume fraction of a given phase, respectively. Here the inelastic effects arise from the application of the generalized Leonov model^{1,2} to simulate the nonlinear viscoelastic response of the matrix phase, Fig. 2(a). It will be shown later in the next section that the choice of so called comparison medium $[L_0]$ is crucial in the success of prediction of both local and average response of the composite. Since only the phase volume averages of the local fields can be inferred from the application HSVP the present approach falls with the category of two-point averaging methods.



Figure 2: a) Stress-strain diagram for epoxy, b) Laminate response - original HSVP, c) Laminate response - modified HSVP

3 RESULTS AND CONCLUSIONS

Although the use of finite element method in the analysis of SEPUCs provides detailed description of the local fields in individual phases it may prove to be prohibitively expensive particularly in the multiscale analysis of complex composite structures. New routes are therefore on demand. A prosperous modeling strategy is offered by the use of HSVP, which considerably saves the computational cost when compared to finite element simulations. When applied in its original format (no change of $[L_0]$ during incremental analysis), however, the method shows substantially stiffer response compared to the "exact" finite element results, Figs 3(a),(b). Erroneous results may be expected even for laminates with heigh fiber volume fraction loaded by uniform strains or stresses, where the assumption of two-point averaging schemes having uniform local fields within individual phases is "exact", Fig. 3(b). With reference to more complex microstructures, Fig. 1(a), this can be attributed to formation of localized shear bands Fig. 4(b) in the composite, which cannot be accurately captured by the simplified model. Similar conclusions were presented also in³.

In order to achieve more realistic response a number of improvements to the Hashin-Shtrikman variational principles are proposed, namely the generalization of the secant method⁴ and the appropriate modification of localization rules.



Figure 3: Mesoscopic response - hexagonal packing

It can be shown that replacing the constant shear modulus of the reference medium by a secant modulus of the matrix phase leads to considerable improvements of the estimate of overall response of the composite, Figs. 2(c), 3(c). While for laminates a perfect match with FE simulations is achieved, 2(c), still stiffer response for hexagonal packing of fibers is evident from Fig. 3(c). However, if the local response is not of the main interest, an adjustment of one of the material parameters of the Leonov model (τ_0 , see¹ for more details) based on numerical rather than laboratory experiments can provide overall response that agrees reasonably well with results derived using the FE method, Figs. 3(c), 4(c).



Figure 4: a) 5-fiber SEPUC, b) Local equivalent strain, c) Mesoscopic response

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