Micromechanical modelling of finite deformation of thermoplastic matrix composites

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Abstract

The prediction of the constitutive behavior of thermoplastic matrix composites from quasi-static up to impact rates demands a detailed understanding of the behavior of the polymeric constituents of these materials; this is due to the pronounced rate dependence of the polymeric matrix. This paper is an attempt at approaching the prediction of finite deformation of thermoplastic matrix composites, using a multi-scale approach in which the fibre and the matrix are separately modelled and combined within a finite element scheme to determine the constitutive response of the test composite. A micromechanical model comprising a finite element implementation of constitutive laws for the fibre and matrix constituents are discussed. The robust formulation for predicting the behavior of the semicrystalline polymer was successfully developed, including the techniques of generating the 3D representative volume element (RVE) of composites as well as prescribing the periodic boundary conditions on the 3D RVE. Finally, the validation studies for predicting the elastic properties of the composite using the Finite Element (FE) methods and the effect of spatial arrangement of the fibre inclusions within the matrix at finite strains are illustrated.

Keywords: Finite element method, thermoplastic matrix composite, micromechanical modelling

1. Introduction

Continuous fibre, thermoplastic matrix, composite materials are attractive for the high volume production, because they combine the good features of manufacturing economics with some of the stiffness, strength and density advantages of the more widely used thermoset matrix composites. They have the potential for industrial and advanced engineering applications, including manufacturing of the components of light-weight cars of the future. However, these materials offer new challenges about prediction of their properties in-use, arising from the pronounced viscoelasticity and plasticity of the matrix polymer, and its sensitivity to the thermal and mechanical history during processing. This study is an attempt at approaching the prediction of the finite deformation of thermoplastic matrix composites in which the modelling approach involves a multi-scale modelling of the composite by tracking deformation from very small strains where linear viscoelasticity conditions apply to finite strains which are dominated by nonlinear viscoelasticity effects. The modelling strategy is divided into microscale and mesoscale levels of analyses. The former deals with a microscale representation of the constitutive models for semicrystalline polymers and the fibre. The later considers the lamina-level representation and modelling of the composite.

In this paper, a finite element implementation of the proposed micromechanical model, at the lamina-level, is emphasised. The test composite used in the study is Plytron, a glass fibre polypropylene matrix composite. The following topics are presented in the

next sections: (a) development of the robust matrix model for semicrystalline polymers; (b) design of a novel method of generating the 3D representative volume element (RVE) of continuous fibre composites; (c) implementation of the periodic boundary conditions (PBCs) and application of single load cases to the 3D RVE; (d) and FE implementation of the chosen homogenization strategy at the lamina-level to predict a nonlinear finite deformation of the composite.

2. Development of the robust matrix model

A robust physically-based constitutive model was developed for modelling the experimentally observed constitutive response for polypropylene; and the test matrix is polypropylene, a semicrystalline polymer. The 1D mechanical analogue for the model is shown in Fig. 1, while Fig. 2 shows the comparison between the model and experimental data for the compression tests on polypropylene. The model prediction is thought to capture accurately the observed experimental response. The matrix modelling principle is an extension to two-process viscoelastic relaxation of a single-mode glass-rubber constitutive model for amorphous polymers[1-3].
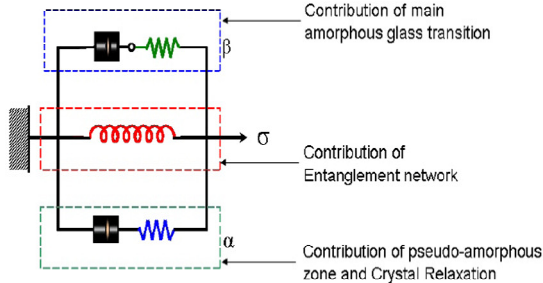

Fig. 1. 1D Mechanical Analogue for modelling of semicrystalline.
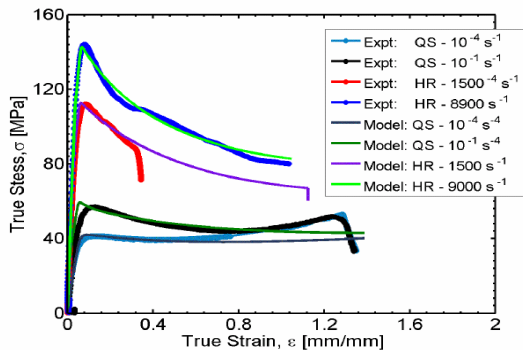

Fig. 2. Comparison of experiments with model prediction for compression tests on polypropylene.

3. A new algorithm for generating 3D RVEs

Having developed a robust matrix model, the next stage of the micromechanical modelling approach is the development of a RVE for the test material. A MATLAB algorithm was developed based on the Monte Carlo Method or Hard Core model[4-6] in which a defined 2D RVE window is populated randomly until a defined volume fraction is achieved. An extra constraint of *periodicity of material* was applied on the generated RVE. For every fibre inclusion that is cut by a boundary wall, the corresponding half of the inclusion is replicated at a corresponding opposite and parallel wall.

Typical RVEs generated using the above approach is shown in Fig. 3 while Fig. 4 shows the strategy for creating a 3D RVE for use in the micromechanical modelling.
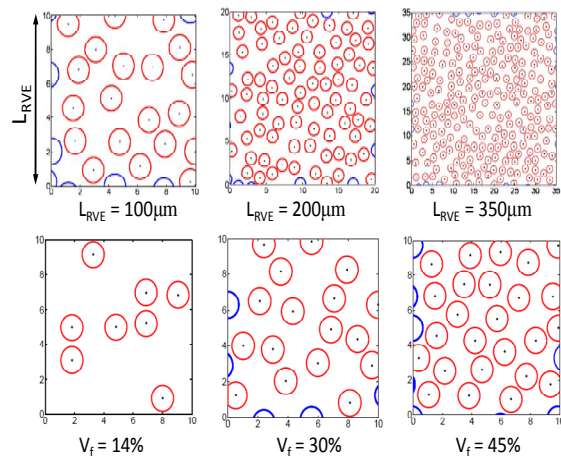

Fig. 3. Typical 2D RVEs generated using the Monte Carlo Algorithm for the different RVE window sizes (LRVE) and different volume fractions (Vf).
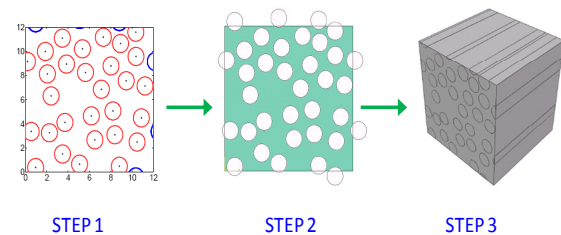

Fig. 4. A three step implementation for creating 3D RVEs. Step 1: 2D RVE generated using Monte Carlo Algorithm. Step 2: Use of Python script within ABAQUS to covert the 2D RVE to the ABAQUS assembly model where white circles are the fibres and a green region is the matrix. Step 3: Extrusion of the 2D model to create a 3D RVE.

4. Implementation of the PBCs on 3D RVEs

Traditionally, the periodic boundary conditions are generally applied to 2D RVEs such that the homogeneous deformation is enforced on the boundary nodes of a given 2D RVE as shown in Fig. 5. This work serves as the first instance where the PBCs are applied to 3D RVEs with the random spatial arrangement of inclusions. This implies applying the homogeneous deformation equations shown in Fig. 6, to all six surface nodes, 8 corner nodes and 12 edge nodes of a 3D RVE.
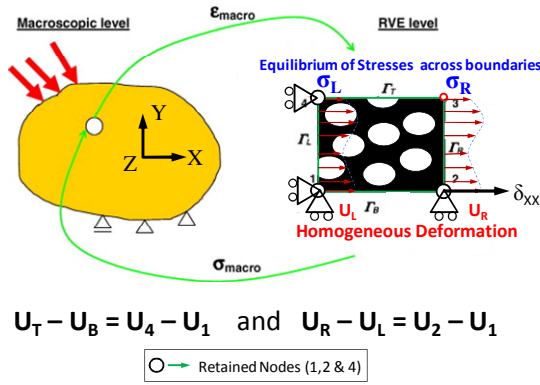

$$U_T - U_B = U_4 - U_1 \quad \text{and} \quad U_R - U_L = U_2 - U_1$$

○ → Retained Nodes (1, 2 & 4)

Fig. 5. A strategy for applying the Periodic Boundary Conditions (PBCs) on 2D RVEs.

$$\mathbf{U}_i^{S_{XPOS}} - \mathbf{U}_i^{S_{XNEG}} - \mathbf{U}^{N_2} + \mathbf{U}^{N_1} = 0$$

$$\mathbf{U}_i^{S_{YPOS}} - \mathbf{U}_i^{S_{YNEG}} - \mathbf{U}^{N_3} + \mathbf{U}^{N_1} = 0$$

$$\mathbf{U}_i^{S_{ZNEG}} - \mathbf{U}_i^{S_{ZPOS}} - \mathbf{U}^{N_4} + \mathbf{U}^{N_1} = 0$$

$$\mathbf{U}^{N_7} - \mathbf{U}^{N_3} - \mathbf{U}^{N_2} + \mathbf{U}^{N_1} = 0$$

$$\mathbf{U}^{N_7} - \mathbf{U}^{N_2} - \mathbf{U}^{N_5} + \mathbf{U}^{N_1} = 0$$

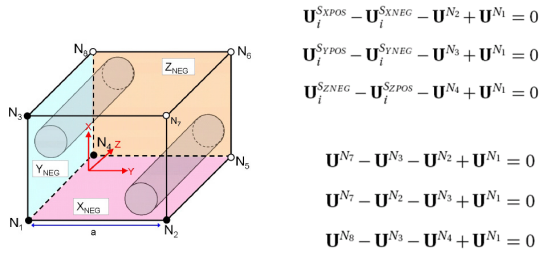$$\mathbf{U}^{N_8} - \mathbf{U}^{N_3} - \mathbf{U}^{N_4} + \mathbf{U}^{N_1} = 0$$

Fig. 6. Strategy for applying Periodic Boundary Conditions (PBCs) on 3D RVEs and list of applicable homogeneous deformation equations for the given 3D RVE domain.

The following shows examples of the simulations based on 3D RVEs of the polypropylene-glass fibre composite where the z-axis corresponds with the fibre direction. Figure 7 presents the logarithmic strain for the compression tests along the x- and y-axes. Figure 8 shows the von mises stress in the z-axis and out-of-plane shear deformation (xy). The logarithmic strain for the out-of-plane (xz) and in-plane (yz) shear deformations is shown in Fig. 9.
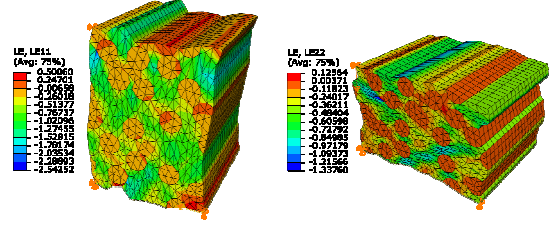

Fig. 7. The logarithmic strain for the compression tests along the x- and y-axes.
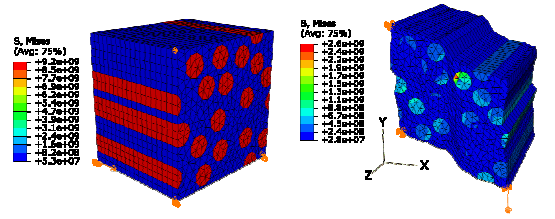

Fig. 8. The von mises stress in the z-axis and out-of-plane shear deformation (xy).
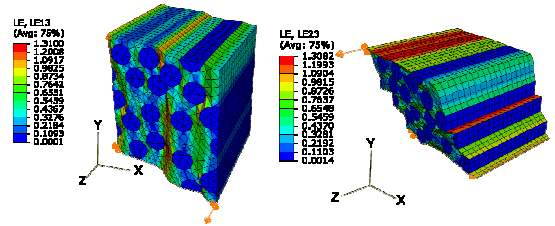

Fig. 9. The logarithmic strain for the out-of-plane (xz) and in-plane (yz) shear deformations

5. Homogenization strategy

In order to derive the constitutive properties of the test composites, the generated 3D RVE implemented with the PBCs has to be used to determine homogenized properties. A homogenization strategy based on the Direct macro-micro relationship[7-11] was adopted in this work. The previous works adopted a 2D RVE where three retained nodes (for the RVE) are used to prescribe any desired load case. This work extended the homogenization strategy above for a 3D RVE such that four retained nodes are used to prescribe the 3D homogeneous deformation for the given RVE.

Consider a typical 3D RVE domain (Ω_{RVE}) such that there exist four retained nodes (N_1, N_2, N_3 and N_4). The coordinate positions for these nodes become: $\mathbf{x_1}$, $\mathbf{x_2}$, $\mathbf{x_3}$, and $\mathbf{x_4}$). The corresponding reactions forces (in 3D) for the four nodes include: f_{N1},

f_{N2}, f_{N3}, and f_{N4}. The formulations for determining the overall stresses and strains at macroscale based on the reaction forces; and coordinate positions of chosen retained nodes are shown below:

$$\sigma_{macro} = <\sigma> := \frac{1}{V}\left\{ x_1 \otimes f_{N1} + x_2 \otimes f_{N2} + x_3 \otimes f_{N3} + x_4 \otimes f_{N4}\right\}$$

$$u_2 = \epsilon_{macro}(X_2 - X_1), \quad u_3 = \epsilon_{macro}(X_3 - X_1), \quad \text{and} \quad u_4 = \epsilon_{macro}(X_4 - X_1),$$
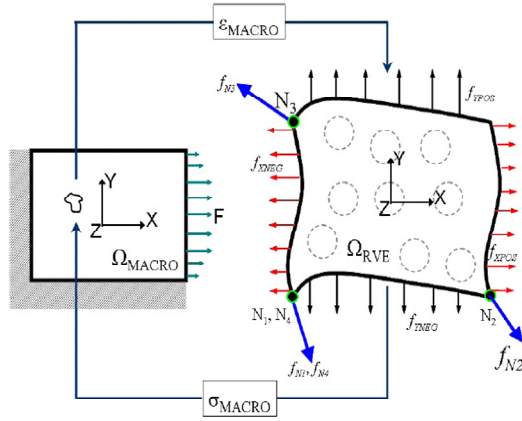

Fig.10. Macro-micro links for an RVE subjected to the periodic boundary conditions.

6. Model predictions

In order to validate the modelling strategy, a boron-aluminum composite of volume fraction 47% was simulated using the above strategy. The experimental data on tests carried out on the boron-aluminum composite [12] and predictions from several prediction approaches were compared with predictions based on this work. One of the other approaches include that attributed to Sun and Vaidya [13] which is an FE method approach using a single-fibre square fibre array 3D RVE. Other approaches are Hashin-Rosen analytical approach based on energy variational principles [14-16], as well as semi-empirical classical laminate theory [17]. This work used two 3D RVEs consisting of (a) one fibre (FEM Small) and size $30\mu m^2$ and (b) 27 fibres (FEM Big) and size $100\ \mu m^2$. Table 1 shows the results of comparison between the two approaches.

In order to determine the elastic properties using the above approach, an optimal RVE window size needs to be determined for the test composite. This is the RVE window size at which there is a convergence of all elastic properties for the given RVE

window. Figure 11 shows the graph of elastic properties against the RVE window size for Young Modulus. Also, model predictions of rate-dependent transverse compression for polypropylene-glass fibre composite are shown in Figure 12 using the above homogenization approach. Again, the effect of spatial fibre arrangement at nonlinear finite deformation is illustrated in Figure 13. This shows the transverse strain (ϵ_{22}) contour plots for six different realizations of a 90x90 μm^2 RVE window tested at 25^0C.
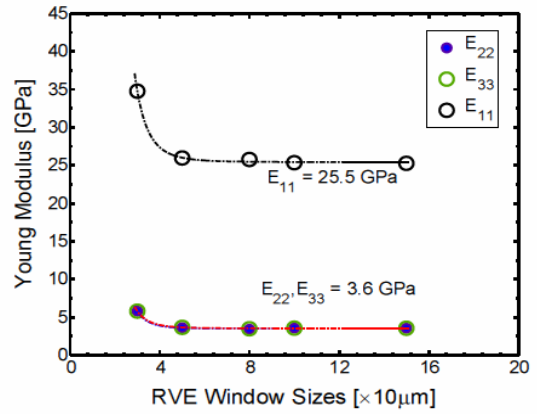

Fig. 11. Variation of predictions of Young Modulus with RVE Window sizes.

Table 1
Comparison of elastic properties of the boron-aluminium composite (v_f=47%) based on different approaches. The fibre axis is along 1-axis and the transverse directions are 2- and 3-axes. Unit: GPa.

Properties	Expt	FEM Big	FEM Small	FEM Sun	Analyt.	Empi.
E_{11}	216	208.7	213.4	214	215	214
E_{22}	140	134.3	141.0	135	139.1 {131.4}	156
E_{33}	-	135.2	141.0	-	-	-
G_{12}	52	52.9	51.9	51.1	53.9	62.6
G_{13}	-	52.8	52.0	-	-	-
G_{23}	-	49.4	45.0	-	54.6 {50.0}	43.6
v_{12}	0.29	0.299	0.300	0.19	0.195	0.20
v_{13}	-	0.299	0.300	-	-	-
v_{23}	-	0.193	0.198	-	0.31 {0.280}	0.31

7. Conclusions

A FE micromechanical model for prediction of the finite deformation of a polypropylene-glass fibre composite is presented. The modelling overview includes (i) development of the robust matrix model,

generation of 3D RVEs, (ii) implementation of PBCs on 3D RVEs, (iii) definition of micro & macro homogenization relationships, and (iv) the model predictions for elastic and finite deformations. The effect of spatial arrangement at the finite deformation suggests that in order to obtain the homogenized responses at such large strains, a large RVE window is required. This presents opportunities for further work.
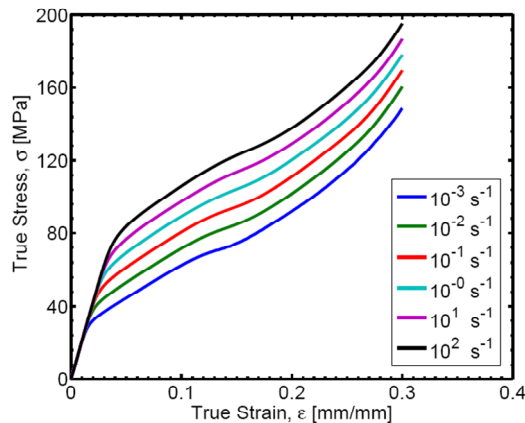

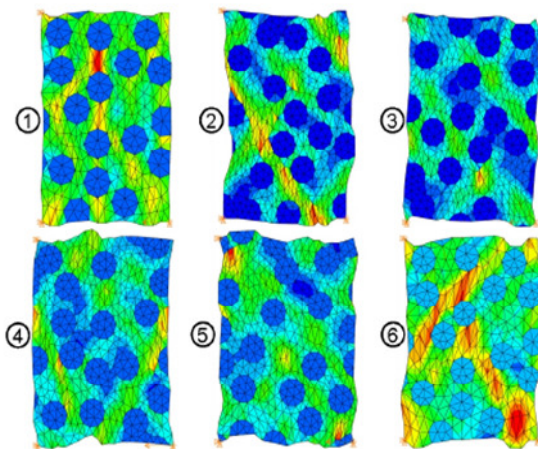Fig.12. Prediction of rate-dependent transverse compression of test composite.

Fig.13. Transverse compression (ε_{22}) contour plots for 6 different spatial arrangements of the test composite.

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