MULTISCALE MODELING OF HIGHLY REINFORCED THERMOPLASTIC COMPOSITE: FROM MICROSTRUCTURAL SIMULATIONS OF THE TRANSVERSE DAMAGE KINETICS TOWARDS ENGINEERING STRUCTURE COMPUTATIONS.

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Keywords: UD composite materials, randomly generated microstructures, X-ray tomography, FE analysis, damage

Abstract
The prediction of mechanical properties of composite materials within engineering structures are of paramount importance for the industry. It is well documented that the microstructure has a significant impact on the material response. In this study, an attempt is made to investigate, using numerical tools, the influence of microstructural variability on UD fibre reinforced thermoplastic composite materials. On the one hand, the porous viscoplastic constitutive model of the matrix is based on *in-situ* tensile tests and X-ray tomography while fibres are considered elastic. On the other hand, an algorithm allowing the generation of periodic composite microstructure cells was implemented. The comparison between statistical and spatial descriptors guarantees a reliable representative volume element of the real composite material under study. Finite Element simulations based on these periodic cells highlighted the effects of the variability of the microstructure on the stress-strain curve, as well as on the evolution of the porosity. An homogenization scheme is subsequently put forward to enable engineering structures computations whilst taking into account microstructural information.

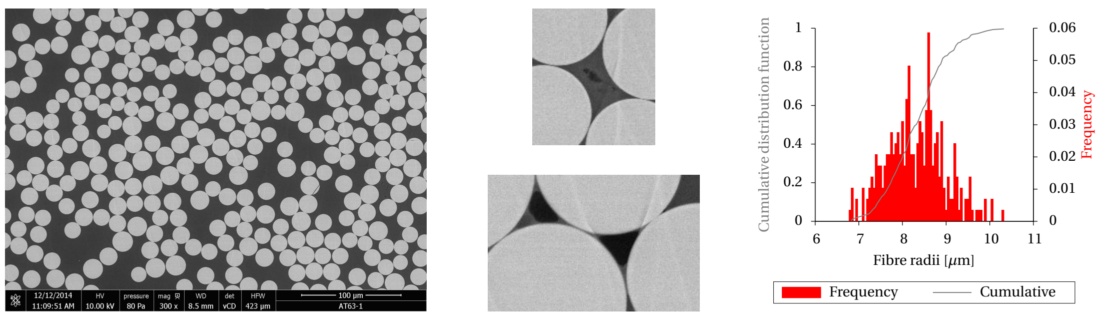
1. Introduction

Owing to their potential to offer high mechanical properties, low weight and a resistance to cyclic loadings, composite materials are increasingly used for high pressure equipments such as stationary or onboard gaseous storage vessels or for pipes. Such engineering structures are submitted to multiaxial stresses which are locally amplified due to the microstructural variability. That is why the prediction of mechanical properties of composite materials within engineering structures are of paramount importance for the industry.

It is well documented that the microstructure has a significant impact on the material response. In this study, an attempt is made to investigate the influence of microstructural variability on UD reinforced thermoplastic composite materials and especially on its transverse behaviour. Indeed, first crackings often occur between fibres and thus affect the load transfer. A numerical approach is chosen to tackle the issue. The composite under study exhibits a high fibre volume fraction (between 60 and 65%) with glass fibres and a PA11 thermoplastic matrix. The material microstructure is accessible via SEM analysis. The behaviour of glass fibres is considered elastic. In-situ tensile tests and X-ray tomography were performed

Excerpt from ISBN 978-3-00-053387-7

on notched PA11 matrix specimens in order to identify a porous viscoplastic constitutive model. The choice was made to describe at best the medium – with representative cells – and the materials – via their constitutive models. The microstructures are generated with inevitably manufacturing-induced attributes that have to be taken into account, such as a random fibre layout, a fibre radius distribution or the presence of porosities (see figure 1).



(a) (b) (c)

Figure 1. (a) Composite under study ; (b) Micro and macro voids ; (c) Fibre radius dispersion

An algorithm allowing the generation of periodic microstructure cells – with high available fibre volume fractions and acceptable computation costs – was implemented in MATLAB and was inspired by the works of Ghossein [**?**]. The comparison between statistical and spatial descriptors guarantees a reliable representative volume element of the real material under study. For this reason, several descriptors available in the literature were added to the code to describe the generated microstructures. Only few of these descriptors were chosen to provide a fine digital representation of the real medium. Following an automated meshing procedure via Gmsh [**?**], Finite Element simulations based on these periodic cells were conducted with the Z-set suite [**?**]. It clearly highlighted the effects of the variability of the microstructure on the stress-strain curve, as well as on the evolution of the porosity in the matrix.

Furthermore, the homogenization step is decisive to go up to the simulation of engineering structures. A numerical homogenization approach based on aforementioned micromechanics computations and optimization technique was used to provide a relevant macroscopic behaviour.

The main steps of the numerical investigation are as follows:

- Material characterization of the bulk matrix which involves an experimental study (whereas fibres will be considered elastic linear and the properties are easily found in the literature) in section 2
- Composite microstructure representation and computations: generation of representative periodic cells, elements of representativness and micromechanical FE simulations in section 3
- Homogenization step in section 4

2. PA11 matrix behaviour characterization through *in-situ* tensile tests and X-ray tomography

2.1. Experimental study

To describe at best our matrix material in the FE computations, *i.e.* while in a confined state between rigid fibres, the chosen constitutive model has to be highly hydrostatic dependent, damage based and well calibrated. This is why several mechanical tests were achieved, on smooth and notched specimen,

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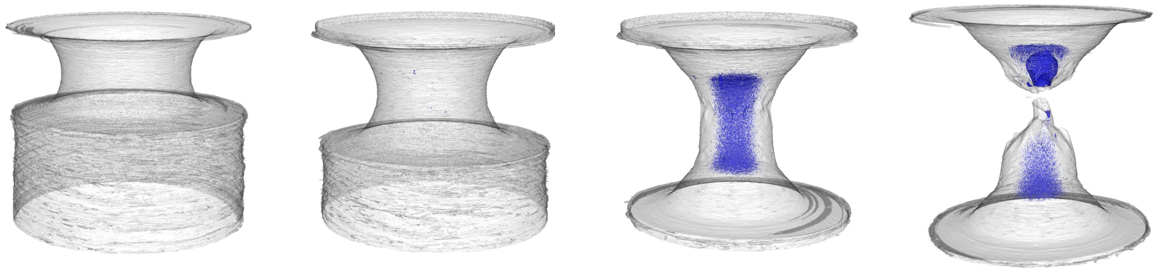
to test various stress triaxiality ratios. Furthermore, damage evolution was monitored on the notched specimen with *in-situ* tensile tests using X-ray tomography (see figure 2). The PA11 polymer subjected to macroscopic uniaxial tension exhibits a void growth which is driven by the stress triaxiality ratio. Besides macroscopic measures such as minimum diameter reduction and notch opening, the void volume fraction and geometrical parameters of individual void were reachable with image analysis on 3D volume data.



(a) Initial stage (b) First visible porosities (c) Before failure (d) *Post-mortem* specimen

Figure 2. X-ray volume rendering of void growth in the PA11 notched specimen and at different steps of the tensile test. The voids are highlighted in blue while the specimen edges are in grey.

2.2. FE modeling

Previous studies on the PA11 [**?** **?**] lead to the use of this modified GTN model which accounts for the elasto-visco-plastic behaviour including isotropic hardening. The porosity f is considered as an internal variable of the model. The initial porosity, f_0, is set to 1% (according to SEM image analysis and X-ray tomography). The chosen constitutive model is implemented under the finite strain formulation available in Z-set.
The constitutive model equations are :

$$\Phi\left(\underset{\sim}{\sigma}, f, \sigma_y\right) = \frac{{\sigma_{eq}}^2}{\sigma_y^2} + 2 f q_1 cosh\left(\frac{q_2 \sigma_{kk}}{2\sigma_y}\right) - \left(1 + q_1^2 f^2\right) = 0 \tag{1}$$

where σ_y is the matrix flow stress. The flow rule and the Norton law equations are as follows:

$$R(p) = R_0 + Q\left(1 - e^{-bp}\right) + A\left(e^{Bp} - 1\right) \qquad \dot{p} = \left(\frac{J(\underset{\sim}{\sigma}) - R}{K}\right)^n \tag{2}$$

The aforementioned macroscopic and microscopic quantities obtained experimentally are used to calibrate – through inverse optimization of the constants above in equations 1 and 2 – the appropriate porous visco-plastic constitutive model.

This type of model can be found for instance in the works of Ricard [**?**] or Cayzac [**?** **?**] on POM and PA6 polymers respectively.

Once the matrix constitutive model is set (with the elastic properties available in the literature), one needs to follow up with composite microstructure representation. Indeed, it is assumed in a first approach that there are no interphase – within the meaning of Meurs works [**?**] – and the matrix of the composite behaves like the bulk material. Furthermore, in accordance with experimental results and as observed by Cayzac [**?**], the damage grows in the matrix and there is no delamination. Hence, the interfaces between matrix and fibres are considered perfect.

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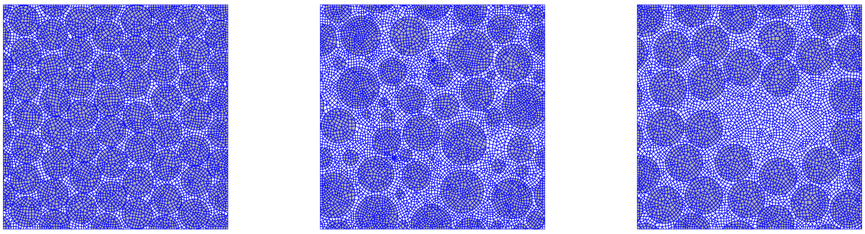
3. Composite microstructure representation

Fibre arrangement in the microstructure plays an important role for the mechanics of the composite. The internal stresses undergone by the fibres and the matrix are locally amplified. The actual loading is complex and the stress state is highly triaxial. A representative cell of the microstructure has to be introduced so as to achieve the computations.

3.1. Microstructure generation

The focus here is on the generation of 2D microstructure cells. Indeed, the transverse cross-section of a UD composite outlines a distribution of disks. Two conditions have to be fulfilled: the disks cannot intersect each other and a certain surface fraction has to be reached. Numerous algorithms can be found in the literature to this extent. However, the works of Ghossein *et al.* [**?**] inspired the present study since it is easier to generate periodic cells at a small computation costs. This method was also implemented in MATLAB and completed with a mesh procedure with Gmsh – since FE computations will follow up the generation of cells – and several statistical and spatial descriptors. Figure 3 exhibits several examples of exotic and available cells with the used method.



(a) $v_f > 80\%$ (b) $\neq$ radii (c) matrix dense zones

Figure 3. Examples of generated meshed cells (the mesh is coarse on purpose for the sake of clarity)

3.2. Statistical and spatial descriptors

To guarantee the representativeness of the generated microstructures, statistical and spatial descriptors are used and are well documented in the literature. Among a non-exhaustive list, the obvious fibre volume fraction, first and second fibre distance distributions, the covariance function or the Ripley's or pair functions can be cited. They can quantititively describe a microstructure, its regularity or disorder, its isotropy or anisotropy, its vacuity or the presence of clusters of fibres. Figure 4 shows two illustrations of a real microstructure and its digitized – but yet representative – counterpart. Integral range can add some relevant information to compute a cell mechanical property with its relative error and for a considered size of cell. The FE computations will be from now on driven with the chosen microstructure, representative of the real medium according to the descriptors.

4. Homogenization strategy

The upcoming step consists of FE simulations on a chosen representative volume element (also called RVE) which is, moreover, periodic. Several elementary micromechanical computations were required to characterize the behaviour of the composite material under complex loading conditions. The results for a base of elementary computations will feed the numerical homogenization which is achieved by optimization.

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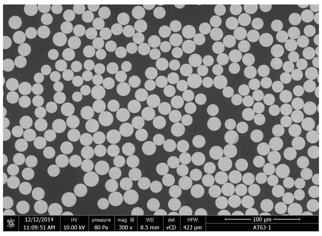
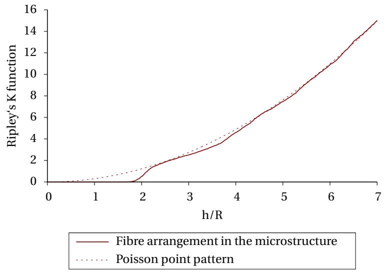
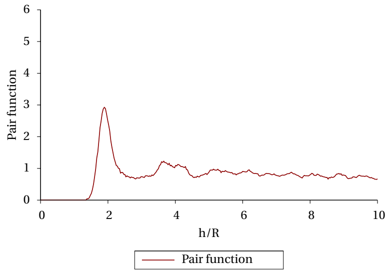


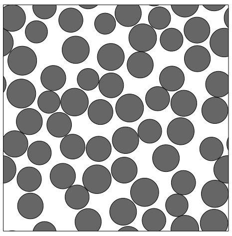
(a) Real microstructure



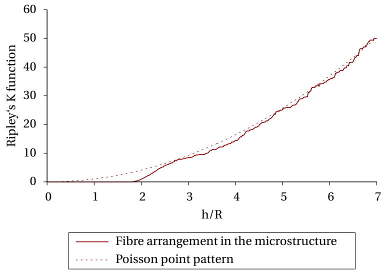
(b) Ripley's function



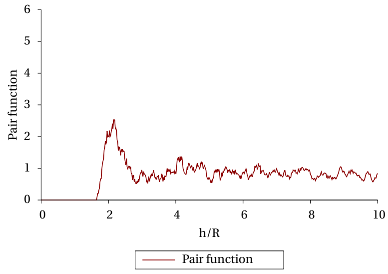
(c) Pair function



(d) Digital microstructure



(e) Ripley's function



(f) Pair function

Figure 4. Real microstructure *vs.* proper representative digital cell

4.1. Elementary micromechanical computations

The cells were built with a periodic mesh. It is supposed that they contain all the necessary statistical information, in accordance with our descriptors and that the ergodic hypothesis holds. Owing to the standard homogenization method, macroscopic (also called overall or averaged) strain E and the macroscopic stress can be introduced, following the Hill [?] and Suquet [?] definitions. These macroscopic quantities come from the microscopic strain $\underset{\sim}{\epsilon}$ and the microscopic stress $\underset{\sim}{\sigma}$ defined by the following equations. By considering a cell with the volume body V and the boundary ∂V:

$$\underset{\sim}{\mathbf{E}} = \langle \underset{\sim}{\epsilon} \rangle = \frac{1}{V} \int_V \underset{\sim}{\epsilon} dV \quad ; \quad \underset{\sim}{\mathbf{\Sigma}} = \langle \underset{\sim}{\sigma} \rangle = \frac{1}{V} \int_V \underset{\sim}{\sigma} dV \tag{3}$$

Special attention is paid on periodic boundary conditions, well documented in the literature [? ? ?] and recommended by Kanit *et al.* in [?], that can be summed up with :

- $\underline{t}$ is anti-periodic, and:

$$\underline{t}(\underline{x}) = \underset{\sim}{\sigma}(\underline{x})\underline{n} \qquad \forall \underline{x} \in \partial V$$

- $\underline{u}_{\#}$ is periodic, and:

$$\underline{u} = \underset{\sim}{\mathbf{E}}\underline{x} + \underline{u}_{\#} \qquad \forall \underline{x} \in V$$

Thus, the periodic formulation makes it possible to prescribe either macroscopic stresses or strains over the cell. The computations are run with the Z-set suite and with finite strain formulation, which is imposed by the matrix model used.

The results exhibit composite local response under simple overall loading and clearly shows high triaxialities undergone locally by the matrix. Damage and voids evolve in these confined zones which lead to failure of the composite.

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4.2. Numerical homogenization through optimization

Since the final goal is to be able to complete engineering structure computations, one needs to work with an homogenized constitutive model of the actual composite. To this extent, the adopted strategy consists in chosing a relevant macroscopic type of constitutive model for the material and computing a numerical optimization.

The macroscopic constitutive model chosen satisfies the following requirements:

- Orthotropic linear elasticity
- Anisotropic plasticity criterion (in this study it is elliptic, similarly to the works of [**? ? ?**])
- Non linear isotropic hardening
- Norton flow rule for the viscoplasticity

The numerical optimization consisted in a minimization of the differences between the stress-strain curves obtained with the full-field results on RVE cells and with this macroscopic constitutive model on a single volume element. Thus, the respective responses have to fit as best as possible for every elementary computations on RVE cells. The figure 5 exhibits the stress-strain responses for the full-field method on the cell (for the six simplier tests which are the traction and shear in each direction) and the counterparts after this optimzation step.

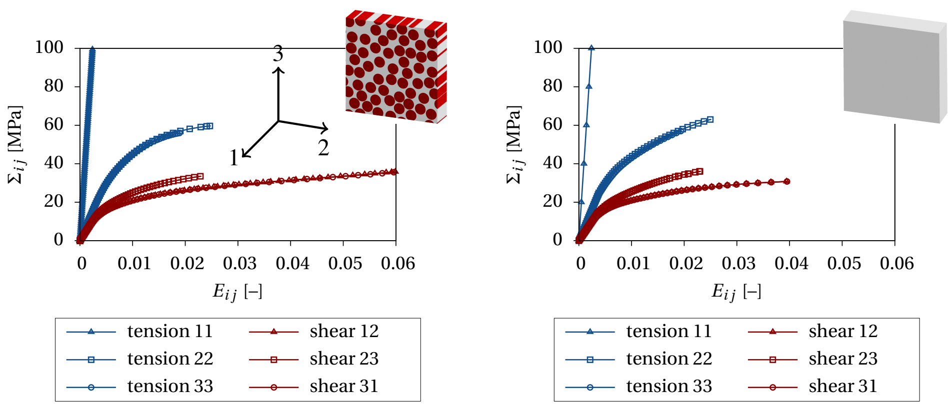

Figure 5. Elementary computations stress-strain curves for a microstructure and the homogenized medium

Computations on complex engineering structures can then be performed using the homogenized equivalent model. Nevertheless, to access the local stresses and strains a relocalisation procedure has to be introduced to assess critical hot spots in the structure.

5. Conclusions

In this contribution, we introduced a numerical methodology able to provide informations about the transverse mechanical response of UD composite materials. To fulfill this goal, the study of microstructures is inescapable to understand the mechanics and kinetics of damage of reinforced thermoplastic composite materials. Our approach relies on generation and FE computations of periodic microstructures where the

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fibre arrangements can be controled to fit the real microstructure and especially the FE models of the constitutive material of the composite – matrix and fibres – are well established.

Using this method, the influence of the variability of the microstructure could be investigated. Each parameter *e.g.* fibre radii dispersion, fibre arrangement, matrix-rich zones, macroporosity or distance between neighbouring fibres could independently be treated. In the present study, mesh generation followed by mechanical computations were achieved but the extension to multiphysics problem such as heat diffusion can also be addressed.

The recent works tackle the scale transitions: from micro to macro. The final goal lies in the industrial effort to accurately predict the properties and evolution of damage of a material within a structure, by advantageously using the materials constitutive models and their microstructures. Further works consist of the examination of the "interphases" (as defined in [**?**]), as well as several experiments on composite materials with in-situ tomographic tests so as to confirm the whole numerical investigation.

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