COMPUTATIONAL MICROMECHANICS ON POLYMER MATRIX COMPOSITES UNDER DIFFERENT ENVIRONMENTS: LONGITUDINAL, TRANSVERSE AND SHEAR PLY PROPERTIES

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Abstract

Qualification of Fiber Reinforced Polymer materials (FRP's) for manufacturing of structural components in the aerospace industry is usually associated with extensive and costly experimental campaigns. The burden of testing is immense and materials should be characterized under different loading states (tension, compression, shear) and environmental conditions (temperature, humidity) to probe their structural integrity during service life. Recent developments in multiscale simulation, together with increased computational power and improvements in modeling tools, can be used to alleviate this scenario. In this work, high-fidelity simulations of the material behaviour at the micro level are used to predict ply properties and ascertain the effect of ply constituents and microstructure on the homogenized ply behaviour. This approach relies on the numerical analysis of representative volume elements equipped with physical models of the ply constituents. Its main feature is the ability to provide fast predictions of ply stiffness and strength properties for different environmental conditions of temperature and humidity, in agreement with the experimental results, showing the potential to reduce the time and costs required for material screening and characterization.

1. Introduction

The traditional way to determine composite ply properties the is through extensive and costly experimental programs which involve material characterization through different levels up to the final global structure. Material testing begins at the ply coupon level and a tremendous effort is needed in order to test materials under tension, compression and shear, to fully certify the different ply properties. Moreover, additional tests might be required under different ageing and environmental conditions, delaying the experimental program in months and years until final material certification. Therefore, predicting mechanical properties and failure mechanisms in FRP has become one of the most active areas in research activities related to material science. The influence of the microstructure and the mechanisms of deformation and fracture of the constituents in the mechanical properties of FRPs has been proven by many authors during recent years. Nevertheless, reliable and accurate failure criteria for composite materials are still under investigation.

Nowadays, computational micromechanics stands out as powerful tool to reliably predict these physical mechanisms as well as the mechanical properties of the composite ply. Numerical simulations of three-dimensional Representative Volume Element (RVE) of the composite microstructure are able to calculate

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lamina properties that can be used in the analysis of laminates [1]. This multi-scale simulation strategy might reduce extensive and costly experimental programs which involve characterization of coupons, panels and subcomponents up to final global structure. However, the characterization of the constituents is not always straightforward, particularly when polymer matrix plastic behavior needs to be captured [2].

In this work a coupled experimental-computational micromechanical framework has been developed to determine the mechanical properties of unidirectional fiber reinforced composites at room temperature under dry atmosphere (RT/DRY) and at elevated temperature and wet atmosphere (HOT/WET). This methodology includes in-situ experimental characterization of matrix and interface [3] performed on the composite cross-section, combined with Finite Elements (FE) numerical simulations of a Representative Volume Element (RVE). Finally, the engineering ply strengths, namely the longitudinal tensile and compressive strengths (X_T and X_C), the transverse tensile and compressive strength (Y_T and Y_C), and the in-plane shear strength (S_L), are predicted using the material properties measured at the micro level.

2. Computational micromechanics modelling

Computational micromechanics is based on the analysis of a statistically representative volume element of the material (RVE) subjected to homogeneous stress states (tension, compression and shear) or temperature increments. The microstructure of the RVE of the unidirectional composite is idealized as a dispersion of parallel and circular fibers randomly dispersed in the polymer matrix. A total number of fibers around 50 is enough to capture adequately the essential features of the microstructure of the material [4] while maintaining reasonable computing efforts. Synthetic fiber distributions statistically equivalent to the real ones are generated for the analysis using the Random Sequential Adsorption (RSA) algorithm [5]. Two-dimensional periodic fiber distributions are generated and then extruded along the fiber direction to achieve the final RVE's of the unidirectional composite material. The periodic RVE's are then discretized using isoparametric wedge and brick fully integrated finite elements for fibers and matrix. Periodic boundary conditions are applied on opposite faces of the RVE's according to the methodology developed by Segurado and LLorca [5]. Simulations are carried out with Abaqus/Standard [6] within the framework of the finite deformations theory taking into account residual thermal stresses due to curing cooldown.

2.1. Constitutive equations

The carbon fibers are modeled in this work as linear, elastic and transversally isotropic solids.

The polymer matrix of the composite material is simulated as an isotropic linear and elastic solid with E_m and ν_m as elastic modulus and Poisson ratio. In addition, the matrix is able to undergo plastic deformations with the possibility of damage by cracking under tensile loads [7]. The damage-plasticity model available in ABAQUS/Standard [6] and schematically illustrated in Figure 1 is used in this work. It is a modification of the Drucker-Prager plasticity yield surface [8] by including a damage variable in order to capture the quasi-brittle behaviour of the polymer under dominant tensile loads. The constitutive equation is based on the yield function proposed by Lubliner et al. [9] including modifications proposed by Lee and Fenves [10] to account for strength evolution under tension and compressive loads.

Fiber-matrix debonding is modelled by means of a surface-based cohesive interaction in ABAQUS/Standard [6]. The cohesive constitutive equation relates the displacement jump across the interface to the traction vector acting on it for cracking under the full range of mode-mixities, as in [11]. Cohesive interactions were used in the model to include the effect of friction occurring after fiber/matrix debonding. The shear stresses caused by friction at the interface are ramped progressively and proportional to the degradation

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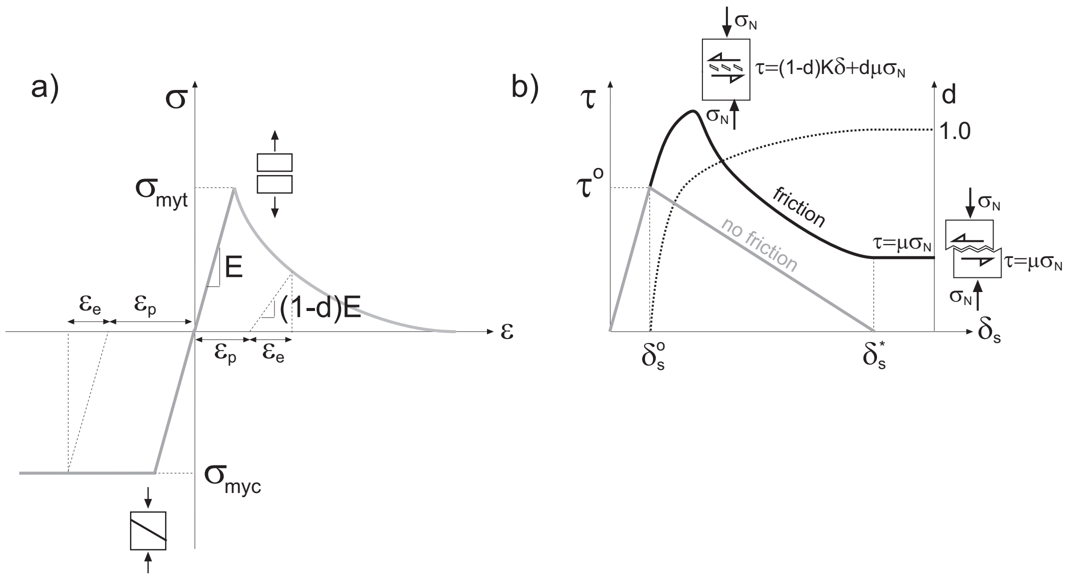

Figure 1. a) Schematic of the uniaxial tensioncompression response of the epoxy matrix according to the damage-plasticity model for quasi-brittle materials, b) Schematics of the shear response of the damage-friction model for fiber/matrix interfaces.

of the interface, and thus, once the fiber/matrix interface is fully debonded, the surface interaction is uniquely governed by a pure Coulomb model. This friction stresses causes an increment of the interface shear resistance proportional to the normal compressive loads applied on it, being μ the constant of proportionality or friction coefficient. It should be mentioned that this affects not only the post-debonding behavior of the interface but also the cohesive response as the friction stresses are ramped with the interface damage variable, as schematically illustrated in Figure 1.

The constitutive model inputs were measured by means of *in-situ* micromechanical tests carried out on environmentally-conditioned composite coupons according to the experimental procedures initially developed by Rodríguez et al. [2, 3], and are gathered in Table 1.

Table 1. Properties of the AS4/8552 material constituents used in the FE simulations.

AS4 carbon fiber properties							
	$E_{f1}(GPa)$	$E_{f2}(GPa)$	$G_{f12}(GPa)$	$G_{f23}(GPa)$	ν_{f12}	$\alpha_{f1}(K^{-1})$	$\alpha_{f2}(K^{-1})$
	231	12.97	11.28	4.45	0.3	-0.9e-6	7.2e-6
8552 epoxy matrix properties							
Condition	$E_m(GPa)$	ν_m	$\sigma_{myt}(MPa)$	β	$\sigma_{myc}(MPa)$	$\mathcal{G}_m(J/m^2)$	$\alpha_m(K^{-1})$
RT/DRY	5.07	0.35	121	29	176	100	52e-6
HOT/WET	4.28	0.35	104	29	152	100	1.5e-6
AS4/8552 fibre/matrix interface properties							
Condition	$\sigma_N(MPa)$	$\tau_T(MPa)$	$\tau_L(MPa)$	$\mathcal{G}_{Ic}(J/m^2)$	$\mathcal{G}_{IIc}(J/m^2)$	$\mathcal{G}_{IIIc}(J/m^2)$	
RT/DRY	42	64	64	2	100	100	
HOT/WET	30	45	45	2	100	100	

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3. Micromechanical simulation of ply behaviour

3.1. Transverse and shear responses

Under pure transverse tension loading, the fracture process is controlled by the fiber/matrix interface debonding, for both RT/DRY and HOT/WET conditions. Cracks start at the fiber poles along the loading direction in those regions where the stress concentrations in the fiber/matrix interface are higher, for instance in a fiber cluster. After failure of the interface, the matrix undergoes severe plastic deformation, accumulating damage until ultimate failure of the matrix ligaments. The final failure of the RVE is produced by the development of a crack perpendicular to the loading axis, as shown in Figure 2. The behaviour is essentially linear an elastic up to failure being the transverse tension strength of the composite strongly controlled by the fiber/matrix interface strength.

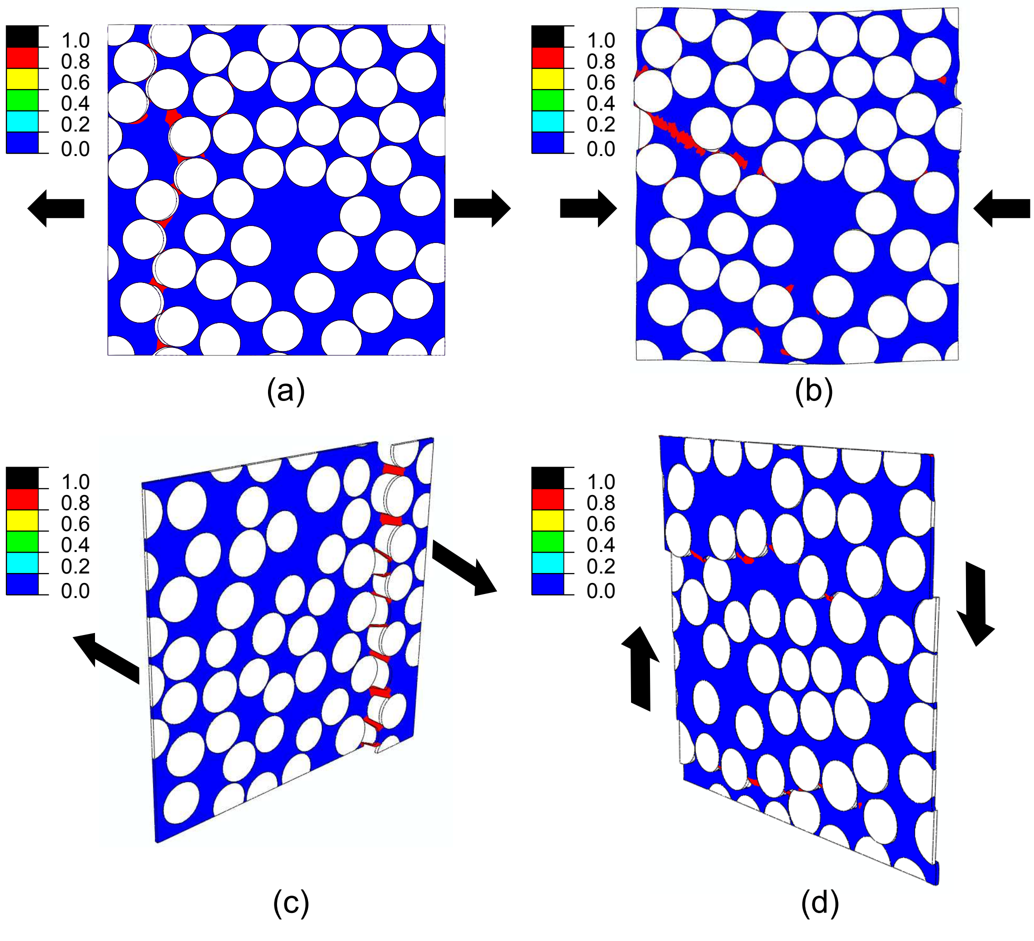

Figure 2. Predicted failure modes in a AS4/8552 ply. Tensile damage for transverse tension (a), parallel shear (c) and perpendicular shear (d). Compression damage for transverse compression (b)

Under pure transverse compression, the final failure of the composite ply takes place by the development of matrix shear bands. However, the fiber/matrix interface plays an important role in the failure initiation process. According to the in-situ nanoindentation tests, the nominal shear strength of the AS4/8552 fiber/matrix interface is lower than the shear strength of the 8552 resin matrix, specially under HOT/WET conditions. If these were the only two mechanisms at play, the simulations show that failure under pure transverse compression would initiate by interface decohesion at the fibre poles and then propagate in the form of a plastic shear band oriented at $\theta_{fr} \approx 47^o$. The introduction of frictional effects in the interaction between fiber and matrix changes this equilibrium between fiber/matrix debonding and matrix

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shear banding. Friction leads to the increment of the interface shearing resistance due to the normal compressive stresses at the interface generated by the thermal and transverse compressive loadings. For significant values of μ, failure under pure transverse compression appears not to be initiated by interface decohesion but directly by shear banding with orientation $\theta_{fr} \approx 56^o$. Values of shear band orientation similar to the later case were reported in previous research works [12] and are supported by experimental data [13] for similar materials. Therefore, it can be concluded that friction plays an important role in the failure process.

When pure shear loading is applied to the RVE, different behaviors are found depending on the shearing direction, parallel or perpendicular to the fibers. If shear is applied parallel to the fibers ($\tau_{||}$), the failure mechanism is dominated by interfacial decohesion or by matrix yielding, depending on the interface strength [14]. In the particular case of the AS4/8552 material studied in this work, the interface strength is slightly lower than the matrix shear limit. Thus, fracture is triggered by interface debonding rather than by matrix plasticity, similarly to the pure transverse tension case. As the interface debonds, the matrix holds progressively shear loads and plastic band deformations are formed. On the other hand, if shear is applied in the plane perpendicular to the fibers ($\tau_{\perp}$), the deformation pattern after matrix yielding is different. Once interface debonding initiates, fiber rotation starts resulting in a gradually stiffer response of the composite material.

The predicted transverse and shear ply properties are summarized in Table 2 and compared with experimentally-obtained data available in the literature [15].

3.2. Longitudinal response

The simulation of the ply longitudinal response requires RVE's with larger dimensions in the longitudinal direction in order to allow the capturing of the respective characteristic deformation mechanisms. In the case of longitudinal tension, the possibility of fibre breakage is taken into account by introducing randomly-located fracture planes in each fiber. The fracture planes are represented by cohesive interaction relations with tensile strengths assigned according to a Weibull distribution based on experimental results [16].

The virtual longitudinal tension process is represented in Figure 3. When the ply is loaded in tension, fibers start to absorb the load uniformly until the weakest fiber-fiber interface fails. At this point, a stress redistribution is produced and the resultant stress concentration is absorbed by the neighboring fibers (A and B) representing a local loading sharing behaviour. More fracture planes fail successively leading to the catastrophic failure of the microstructure (C and D). It is found that the RVE size is large enough to capture the influence of the Weibull distribution in the fiber fracture strength and, hence, in the final failure of the ply.

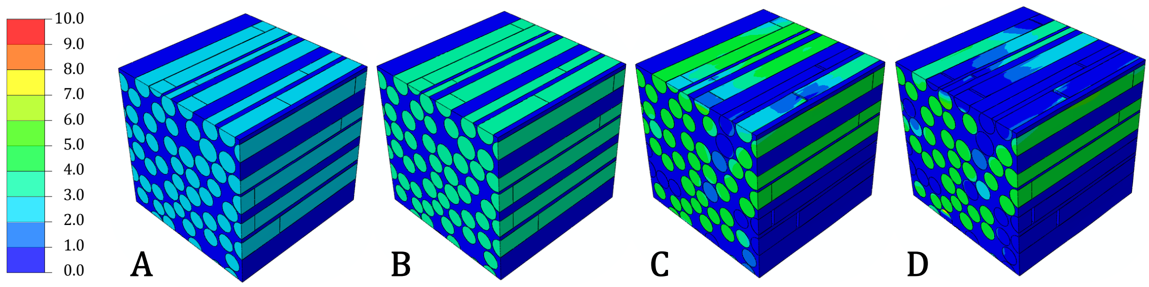

Figure 3. Evolution of equivalent von Mises stress in the RVE under longitudinal tension

Under HOT/WET conditions, the elastic response of the lamina is similar to the one obtained for RT/DRY.

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The influence of polymer and interface enhances the non-linear behavior. However, the stiffness of the carbon fiber, not affected by the moisture uptake, and the large volume fraction govern the ply response, leading to a X_T similar to the one found under RT/RDY conditions. In both cases, the values are in good agreement with experimental results found in the literature [15] and gathered in Table 2.

In the case of longitudinal compression X_C, the initial fiber misalignment,ϕ_0, is clearly the governing parameter. For this reason, a fiber misalignment distribution, $f(\phi_0)$, and a corresponding sensitivity function $X_C(\phi_0)$, which represents the evolution of X_C for different values of ϕ_0, must be considered in order to have a good prediction of the ply strength using the RVE approach. The first simulations are done using a sinusoidal-shape RVE with $\phi_0 = 3^o$, as represented in Figure 4. The model captures the fiber kinking failure mechanism and is able to predict post load-peak features such as the kink band angle and width. However, the simulations require large computational resources and are not practical for fast predictions and parametric studies. To overcome this limitation, a faster 3D single fibre model is developed which is able to predict the kinking load, hence the sensitivity function, with similar accuracy to its multi-fibre counterpart, although it cannot capture the post-peak features.

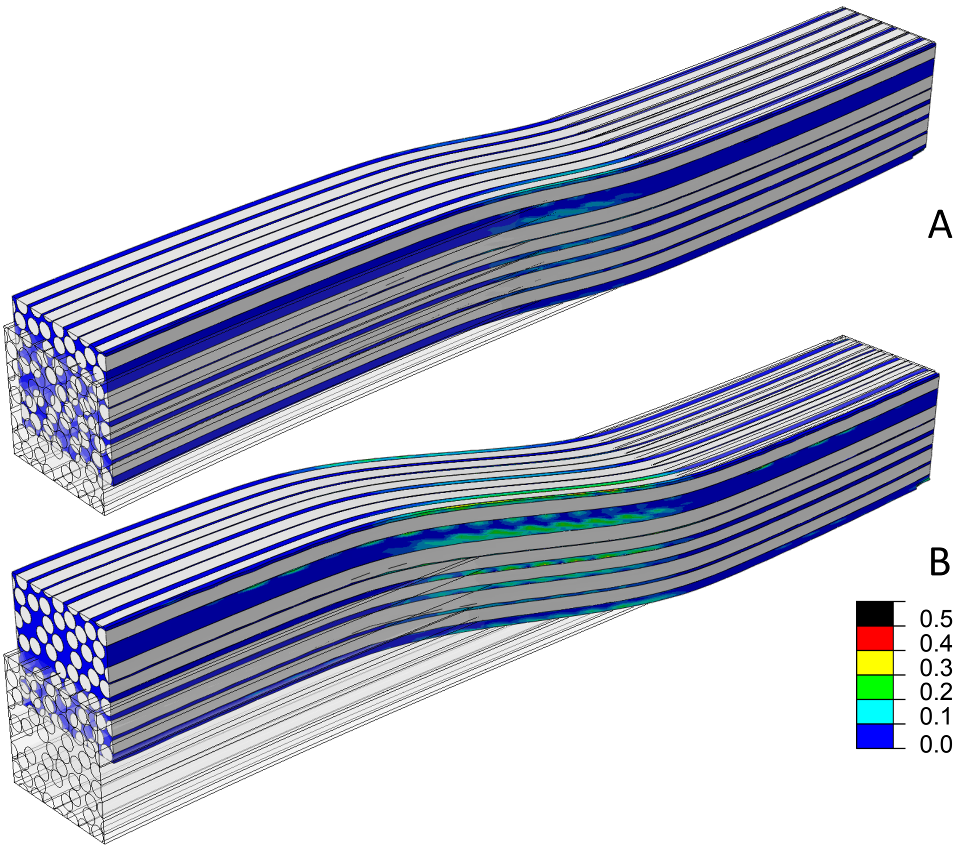

Figure 4. Predicted plastic strain in AS4/8552 ply under RT/DRY conditions. Points A and B correspond to peak load and fully developed kink band, respectively.

The ply compression strength is predicted using the method developed by Barbero [17], which states that the applied load function, $\bar{\sigma} = X_C(\phi_0) \cdot F(\phi_0)$, represents the effective stress times the area of fibers that remain unbuckled. Compared to the experimental values in the literature [15], the results found overestimate the X_C in the order of 20%. Lee and Soutis [18] demonstrated that there is a strong size effect in FRP laminates under longitudinal compression, i.e. there is an intrinsic strength reduction when increasing the thickness of the sample, due to a larger fiber misalignment and void content. In order to account for this size effect, they proposed the empiric relationship $X_{C,ply} = X^{st}_{C,ply} t^{-\alpha}$ for a similar material

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system, wherein $X^{st}_{C,ply}$ is the measured compressive strength of their baseline 2mm thick specimen, t is the thickness of the current specimen and α is the empirically-determined parameter equal to 0.25. Using this model, the predicted compressive strength of a AS4/8552 ply under both RT/DRY and HOT/WET conditions remarkably agree with experimentally-obtained results [15] which are gathered in Table 2.

4. Discussion and conclusions

The predicted properties of a AS4/8552 ply under RT/DRY and HOT/WET environment conditions are gathered in Table 2. The reported numerical results are the average of five different random realizations and are in good agreement with experimentally-obtained average ply properties reported in the literature [15], specially for RT/DRY conditions.

Table 2. Numerically-predicted vs. experimentally-obtained AS4/8552 ply properties for RT/DRY and HOT/WET conditions (* provided by Hexcel)

	RT/DRY		HOT/WET	
Property	Micromechanics	Literature [15]	Micromechanics	Literature [15]
E_2(GPa)	9.2	9.6	8.3	8.4
G_{12}(GPa)	4.8	4.8	3.1	2.3
$X_T(MPa)$	2208	2062 (2207*)	2158	1964
$X_C(MPa)$	1374	1397 (1531*)	1080	1036
Y_T(MPa)	61±3	63.9	36±2	24.1
Y_C(MPa)	290±30	268.0	141±7	136.0
$S_L^{0.2\%}$(MPa)	55±1	55.2	34±1	23.2
$S_L^{5\%}$(MPa)	88±3	91.6	55±3	38.0

Hence, this paper suggests that virtual ply characterization tests, based on reliable properties of the micro-constituents, can replace the physical experiments, at least for material screening purposes. These virtual tests provide full control of the composite microstructure and constituent properties, allowing microstructural optimization to be performed in the future [19]. Moreover, the influence of the microstructure and its microconstituents in the failure mechanisms can be assessed by means of parametrical analysis, leading to the development of micromechanical based failure criteria with physical soundness that can be compared to the state-of-the-art Puck and LaRC predictions.

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