MICROMECHANICAL MODELING OF THE EFFECT OF HOT-WET CONDITIONS ON THE MECHANICAL BEHAVIOR OF COMPOSITE MATERIALS

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Abstract

The mechanical behavior of a polymer reinforced composite material under mechanical and environmental conditions was simulated by means of a computational micromechanics approach. Within this framework, a representative volume element RVE of the composite material is discretized using three dimensional finite elements and the microstructure taken into account explicitly –including fiber-matrix topology-. The simulation strategy takes into account the competition of the different failure mechanisms experimentally observed for unidirectional composite laminas such matrix plasticity and interface decohesion.

1 Introduction

Carbon Fiber Reinforced Polymer Composites CFRP are made up of two phases with a very large mismatch in their mechanical properties. The carbon fibers are stiff, strong and brittle while the polymers matrices are compliant and soft undergoing considerable deformations before fracture under specific loading conditions. Therefore, the mechanical behavior of the composite material depends on the loading conditions which trigger different failure modes dominated by fibers, matrix and interfaces. In the current situation, there is a missing link between the properties of the constituents of the composite material and the macroscopic performance. This affirmation is more evident when studying the in-service behavior of composite materials such as the effect of the temperature and water uptake on their mechanical performance. In those cases, the water absorbed by the composite acts as a plasticizer of the polymer matrix which became softer while the interface between the fibers also is been degraded.

The material models in the literature for hot/wet environmental ageing are still purely phenomenological and rely on a number of macroscopic parameters whose physical meaning is not always well established and which are fitted with experimental results. This panorama is starting to change through the application of computational micromechanics to predict the constitutive response of fiber reinforced composites [1]. In this approach, the mechanical response of the material is obtained from the numerical simulation of a representative volume element (RVE) of the composite lamina, which explicitly takes into account the details of the microstructure, constituent properties, volume fraction, fiber distribution, etc.

2 Computational Micromechanics

The RVE of a UD lamina microstructure is a prism, with a square section of dimensions L×L in the 23 plane perpendicular to the fibers. The fiber centers in this plane were generated randomly and sequentially using the random sequential adsortion algorithm, as described in [2,3,4,5]. The RVE is encomprised a few dozens of circular fibers included within the RVE with the same volume fraction of a carbon/epoxy composite material. It was assumed that the lamina microstructure was given by an indefinite translation of this RVE along the 2 and 3 axes to eliminate surface effects and, thus, the fiber positions within the RVE kept this periodicity condition, Figure 1b). Finally, the RVE was extruded along the fiber axis to obtain the three-dimensional prism, Figure 1 a). This prismatic RVE was discretized for the analysis with the finite element method. The model volume (matrix and fibers) was meshed using modified quadratic 10-node tetrahedral (C3D10M in Abaqus) using an adaptive automatic meshing algorithm. Interface failure was taken into account by inserting cohesive elements between matrix and fibers throughout the model. The cohesive elements are compatible with C3D10M solid elements in Abaqus and were programmed as a UEL subroutine.

Periodic boundary conditions were applied to the RVE surfaces to ensure continuity between neighboring RVEs (which deform like jigsaw puzzles). Different loading conditions can be analyzed by imposing displacement U_1, U_2, U_3 of the master nodes and solving for the reaction forces necessary.

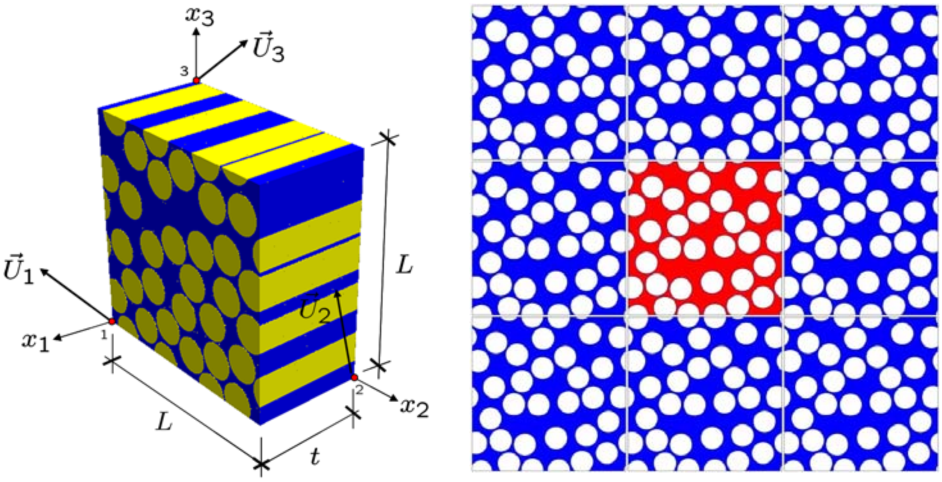

Figure 1. a) Representative volume element of the lamina microstructure RVE, b) Periodic microstructure of the material.

Carbon fibers were modeled as linear, elastic transversally isotropic solids. The epoxy matrix was assumed to behave as an isotropic, elasto-plastic governed by the Drucker-Prager criterion and the total matrix strain was given by the addition of the elastic and plastic strain components. The Drucker-Prager criterion assumes that yielding takes place when

$$\phi = \sqrt{3J_2} - d - \frac{I_1}{3}\tan\beta = 0$$

where I_1 stands for the first invariant of the Cauchy stress tensor, σ_{ij}, and J_2 for the second invariant of the deviatioric part of the Cauchy stress tensor. The elasto-plastic behaviour of the material is thus characterized by the two elastic constants E and ν (assuming isotropic behavior) and the two parameters which dictate the onset of plastic deformation, namely the cohesion d and the friction angle β, which controls the pressure-sensitivity of the material. The interface debonding is modeled by inserting cohesive elements which are controlled by the two basic parameters, the interface strength t_c –stress at which the cohesive elements start to open- and the fracture energy Γ_i, or energy necessary to fully debond the interface.

3 Experiments

The in-plane shear response of a unidirectional carbon fiber reinforced polymer was measured by using $[\pm 45^o]_{ns}$ laminates coupons subjected to plain tension. The coupons were first subjected to hot/wet ageing in environmental chambers at specific temperature and relative humidity conditions until fully saturation was attained. After ageing, the specimens were tested at different temperatures to ascertain the effect of the water uptake on the mechanical response under in-plain shear loadings. The in-plane shear stress-strain curve showed three different regimes. The first one is related with the elastic behavior of fiber and matrix and this early ends with the progression of a non-linear region dominated by the shearing of the epoxy matrix. After critical point, fiber matrix interface decohesion takes place and trigger matrix cracking across the ply and the behavior of the coupon specimen is dominated by the interaction between matrix cracking and interply delamination. Finally, the stress carried by the composite increased monotonically until the failure. This later behavior was controlled mainly by the elastic behavior of the fibers which progressively rotate as the shear deformation takes place.

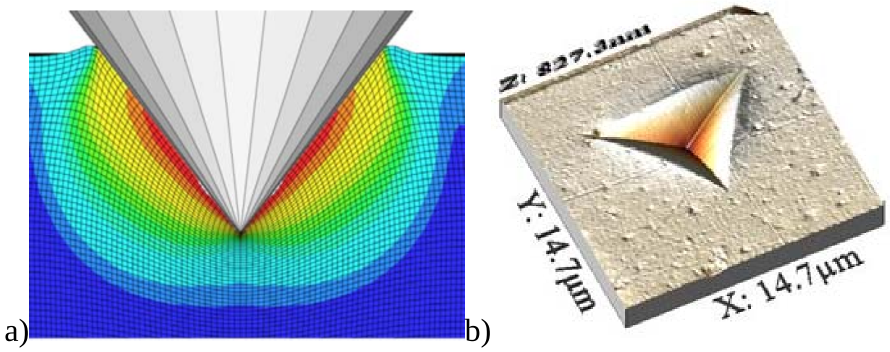

Figure 2. a) Berkovich indentation performed in resin pocket, b) Detailed simulation of the indentation process by finite element.

Micromechanical parameters were measured through instrumented nanoindentation. To this end, sections of the composite coupons were first cut perpendicular to the fibers and polished for indentation purposes. The matrix rich regions were used to characterize the mechanical behavior of the matrix. The load-displacement curves in combination with a detailed simulation of the process, Figure 2, were used to infer the mechanical properties of the matrix namely the matrix cohesion d and the friction angle β. A detailed explanation of the process of extraction of mechanical parameters of a Drucker-Prager material from indentation load-displacement curves can be found in [6].

On the other hand, push-in tests were used to debond individual fibers and extract the cohesive parameters required for the simulation [7]. The mechanical parameters, interface strength t_c and fracture energy Γ_i can obtained by reverse analysis using a detailed finite element simulation of the indentation area, Figure 3a). The experimental load-displacement curves were obtained from indentation of individual fibers using a nanoindentor (MTS XP NanoIndentor). The effect of water absorption on the mechanical parameters of matrix and fiber/matrix interfaces was addressed by means of these combined experimental/simulation framework.

The micromechanical parameters were used as inputs for the numerical simulation of the RVE according to the model presented in section 2. In-plane shear loading was introduced and the load-displacement curves obtained in the simulation allowed the computation of the stress-strain curve of the unidirectional composite. The effect matrix yielding (and the plasticizer effect of the hot/wet ageing) and fiber-matrix interface decohesion on the in-plane shear behavior of carbon-fiber reinforced composites was also addressed.

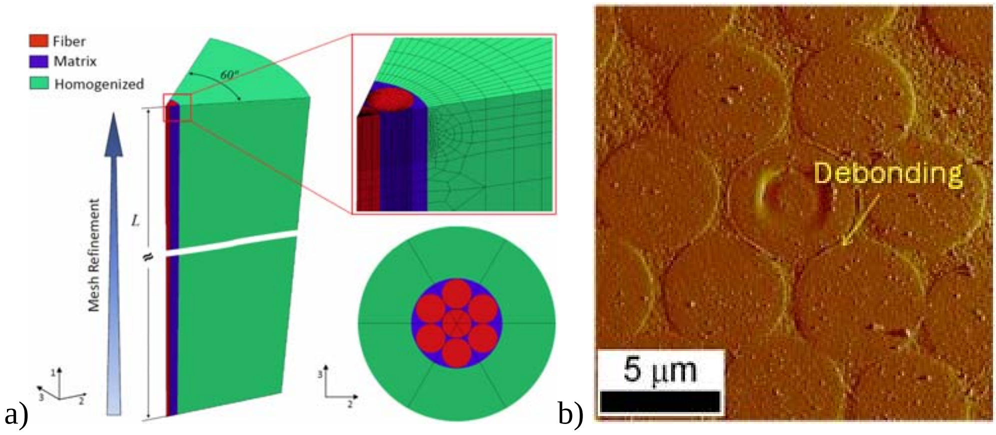

Figure 3. a) Finite element model used to simulate the push-in test in unidirectional composites, b) Atomic Force Microscope image of the indented fiber visualizing debonding.

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References

[1] J. LLorca, C. González, J.M. Molina-Aldareguía, J. Segurado, R. Seltzer, F. Sket et al., Multiscale modeling of composite materials: a roadmap towards virtual testing, Adv Mater, **23** (2011), pp. 5130–5147

[2] C. González, J. Llorca, Mechanical behavior of unidirectional fiber-reinforced polymers under transverse compression: microscopic mechanisms and modeling, Compos Sci Technol, **67** (2007), pp. 2795–2806

[3] E. Totry, C. González, J. Llorca, Failure locus of fiber-reinforced composites under transverse compression and out-of-plane shear, Compos Sci Technol, **68** (2008), pp. 829–839

[4] E. Totry, C. González, J. Llorca, Influence of the loading path on the strength of fiber-reinforced composites subjected to transverse compression and shear, Int J Solids Struct, **45** (2008), pp. 1663–1675.

[5] E. Totry, J. M. Molina-Aldareguia, C. González, J. Llorca. Effect of fiber, matrix and interface properties on the in-plane shear deformation of carbon-fiber reinforced composites. *Composites Science and Technology*, **70**, 970-980, 2010.

[6] M. Rodríguez, J.M. Molina, C. González, J. LLorca, Determination of the mechanical properties of amorphous materials through instrumented nanoindentation, Acta Materialia, **60**, (2012), pp 3953–3964

[7] J. M. Molina-Aldareguía, M. Rodríguez, C. González, J. Llorca. An experimental and numerical study of the influence of local effects on the application of the fibre push-in test. Philosophical Magazine, **90**, 2010.