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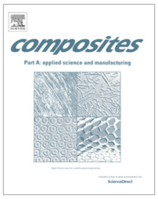

Computational micromechanics of the transverse and shear behavior of unidirectional fiber reinforced polymers including environmental effects

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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 behavior at the micro level are used to predict ply properties and ascertain the effect of ply constituents and microstructure on the homogenized ply behavior. 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

Fiber Reinforced Polymers (FRPs) are nowadays extensively used in applications where good mechanical properties are required in combination with weight savings. However, despite all existing information and current knowledge about these materials, the accurate prediction of the failure stress of composite materials and structures has been an elusive task due to the complexity of the failure mechanisms involved.

Various phenomenological and physically-based models have been proposed, whose input parameters have to be obtained through costly and time-consuming experimental campaigns for each material system [12,22]. Results obtained for a given unidirectional FRP system cannot be directly extrapolated to other configurations with different fiber volume fraction or constituent properties, leading to a massive investment for their physical characterization. This is the case of material qualification for the aeronautical industry, where the whole process can last well over two years due to the required tests under different aging and environmental conditions.

Computational micromechanics (based on Finite Elements Analysis) offers a novel approach to understand the deformation and fracture mechanisms in materials engineering. In the case of unidirectional fiber-reinforced composites, it has demonstrated high accuracy in the prediction of the mechanical behavior, including fracture mechanisms under complex multiaxial loading cases [31,39,41]. Numerical simulations of Representative Volume Elements (RVE's) of the composite microstructure are useful to predict homogenized lamina properties, in close agreement with experimental data [8], and to provide the necessary input data for mesomechanical analysis at the laminate level. This bottom-up multi-scale simulation approach might lead in the future to a drastic reduction of the current costs associated with properties screening and material characterization programs [26]. In addition, computational simulation of micromechanical RVE's can be used to reproduce experimental stress conditions rather difficult to impose experimentally in laboratory, such as biaxial or triaxial stress states. Moreover, the influence of the microstructure and the constituents properties in the failure mechanisms can be addressed by means of parametric studies. All these efforts can lead in the future to the development of micromechanical-based failure criteria with

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physical soundness, a clear advance in the state-of-the-art, e.g. Puck [36], LaRC [14] and Catalanotti [10] models.

Following previous research works [40,45], herein detailed information of the microstructure (fiber diameter distribution, volume fraction, fiber clusters and resin pockets) is captured and included in a computational model of a unidirectional lamina (UD). Several strategies to determine micromechanical parameters by fitting against experimental results at the ply level, rather than measuring them with independent tests at the micro level, were developed in the past [30,35]. In this work, the behavior of the constituents is obtained from micromechanical experiments on the material constituents performed under different environmental conditions. The measured properties are inputs of the constitutive equations of matrix and fiber/matrix interfaces. The RVE is submitted to homogeneous stress states to determine the material failure envelope in the $\sigma_{22} - \tau_{12}$ plane under different environmental conditions, including the pure mode ply strengths, namely transverse tension strength (Y_T), transverse compression strength (Y_C), and longitudinal shear strength (S_L). The model shows the importance of capturing adequately the competition between the different failure mechanisms, fiber/matrix debonding and matrix failure, operating at the same time when the material is subjected to mechanical and environmental loads.

This introduction is followed by the description of the computational micromechanics framework, i.e. of the constitutive equations used to simulate matrix, fiber and interfaces, as well of the RVE generation procedure and the subsequent construction of the FE models with the specific loading conditions. The procedures used to characterize the basic ply constituents and model input parameters are explained then. The results of the uniaxial and biaxial loading simulations performed on the Hexcel carbon/epoxy AS4/8552 material (fiber volume fraction: 60%; cured ply thickness: 0.184 mm) are presented and compared with experimental results. The main advantage of selecting this well-known pre-impregnated material system is that most of its ply properties are directly provided by prepreg manufacturer or found in the literature since it has been widely used in the aeronautical industry and subject of research, e.g. [27,29].

The experimental-computational approach presented in this work constitutes a good complement to the experimental characterization campaigns of composite materials to reduce time and costs associated and providing fast screening capabilities to improve material downselection for a given engineering application.

2. Computational micromechanics model

2.1. RVE model set-up and simulation

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 [18] while maintaining reasonable computing efforts. Triple size RVE's were generated and the results compared to ensure that the selected number of fibers did not influence significantly the model predictions and, thus, the RVE can be considered statistically representative.

Synthetic fiber distributions statistically equivalent to the real ones are generated for the analysis. To this end, several strategies are available in the literature [32,43,45] being the Random Sequential Adsorption (RSA) algorithm [40], probably, the most popular due to the easiness to achieve large volume fraction of fiber reinforcement. In this work, the RSA algorithm was compared with the Nearest Neighbor Algorithm (NNA) developed by Vaughan and McCarty [45] using the relevant microstructure statistical information obtained from micrographs of the unidirectional ply cross section. As shown in Fig. 1, the results revealed well-distributed fiber microstructures without significant fiber clustering or matrix rich regions. Hence, it can be concluded that both algorithms deliver similar microstructures.

Considering its reliability and computing speed, the RSA algorithm was preferred in this work. Two-dimensional periodic fiber distributions were generated with the RSA algorithm and extruded along the fiber direction to achieve the final RVE's of the unidirectional composite material. The periodic RVE's were then discretized using isoparametric wedge and brick finite elements for fibers and matrix with full integration at Gauss points (C3D6 and C3D8, respectively, in Abaqus [13]). Typically, each RVE contains approximately ≈40,000 elements representing a discretization fine enough to capture the large stress gradients between neighboring fibers. Node positions on opposite faces of the RVE's are identical in order to apply periodic boundary conditions according to the methodology developed by Segurado and LLorca [40]. Simulations were carried out with Abaqus/Standard within the framework of the finite deformations theory with the initial unstressed state as reference.

The RVE's were initially subjected to a homogeneous temperature drop of $\Delta T = -160\,^\circ\mathrm{C}$ from the curing (180 °C) to room temperature (20 °C), hence generating a residual stress state in the material before mechanical loading. For the sake of simplicity, the effects of temperature dependence of thermoelastic constants of the constituents or viscous phenomena as stress relaxation, etc. were taken into account in the simulations. In a second step, homogeneous stress states were introduced by applying the appropriate displacements to the master nodes linked with the periodic boundary conditions [18]. The displacement and reactions of these master nodes were used to determine the stress–strain curves under transverse, shear and combined loads, and to derive the corresponding material stiffness and strength properties.

2.2. Constitutive equations

Carbon fibers are modeled in this work as linear, elastic and transversally isotropic solids. The anisotropy is taken into account by defining five independent elastic constants ($E_{f1},\ E_{f2},\ \nu_{f12},\ G_{f12},\ G_{f23}$) and two different thermal expansion coefficients ($\alpha_{f1},\ \alpha_{f2}$).

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. This approach has been adopted by other researchers in the literature [3,9,30,47] as it represents a realistic behavior of a polymer [16]. The damage-plasticity model, available in ABAQUS/Standard [13] and schematically illustrated in Fig. 2, is a modification of the Drucker–Prager plasticity yield surface [15] by including a damage variable in order to capture the quasi-brittle behavior of the polymer under dominant tensile loads. The constitutive equation is based on the yield function proposed by Lubliner et al. [28] including modifications proposed by Lee and Fenves [25] to account for strength evolution under tension and compressive loads. The yield function defined in terms of the I_1 and J_2 invariants of the stress tensor is

$$\Phi(I_1, J_2, \sigma_I, \beta, \alpha) = \frac{1}{1-\alpha}\left(\sqrt{3J_2} + \alpha I_1 + B\langle\sigma_I\rangle\right) - \sigma_{myc} = 0 \qquad (1)$$

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