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Computational micromechanics evaluation of the effect of fibre shape on the transverse strength of unidirectional composites: An approach to virtual materials design

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ABSTRACT

Computational micromechanics of composites is an emerging tool required for virtual materials design (VMD) to address the effect of different variables involved before materials are manufactured. This strategy will avoid unnecessary costs, reducing trial-and-error campaigns leading to fast material developments for tailored properties. In this work, the effect of the fibre cross section on the transverse behaviour of unidirectional fibre composites has been evaluated by means of computational micromechanics. To this end, periodic representative volume elements containing uniform and random dispersions of 50% of parallel non-circular fibres with lobular, polygonal and elliptical shapes were generated. Fibre/matrix interface failure as well as matrix plasticity/damage were considered as the fundamental failure mechanisms operating at the microscale under transverse loading. Circular fibres showed the best averaged behaviour although lobular fibres exhibited superior performance in transverse compression mainly due to the higher tensile thermal residual stresses generated during cooling at the fibre/matrix interface.

1. Introduction

Polymer matrices reinforced with high performance fibres or FRP's are preferred candidates in structural applications where the strength to weight ratio leads the structural design process. One of the main drawbacks regarding the use of these materials is their complex mechanical behaviour, hardly predictable, which depends on the constituents properties, fibres, matrix and interfaces, as well as their spatial distribution within the material. Manufacturing conditions also play an important role and are responsible for the generation of defects in the form of voids, interfacial debonds, resin pockets or dry fibre areas which are considered detrimental for the final performance of the material. The mechanical response of FRP's is, obviously, strongly influenced by the mechanical properties of the high performance fibres used (carbon, glass, aramid, etc.) albeit their spatial distribution, tow architecture and cross section governs the basic deformation and failure mechanisms [1].

Since the discover of high-performance carbon fibres, the composite production process has been optimized to maximize their intrinsic mechanical, thermal and electrical properties. Despite these efforts, the morphology of the reinforcing fibres has barely evolved since its discovery and most developments in this field were kept at a basic research level due to major manufacturing difficulties [2,3].

Pitch-based carbon fibres with different non-circular cross section have been extensively studied by Edie and Dunham [4]. This research group determined the main manufacturing parameters as the mesophase pitch viscosity, winding speed and temperature controlling the fibre properties using a lab-scale set-up. Trilobal and octolobal fibres were obtained from the extrusion of the filaments from different cross section spinnerets [5,6]. From a mechanical point of view, trilobal and round fibres respond differently to increasing process temperatures (i.e. carbonization). Trilobal fibres exhibited a higher longitudinal elastic modulus and tensile strength than standard circular ones (744 GPa and 2.72 GPa, respectively being 1900 °C the carbonization temperature) [5,6]. Comparing to the radial fibre texture, typical of carbon fibres spun from mesophase pitch, the microstructure of trilobal carbon fibres does not emanate radially from a centre point, but

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instead grows up from three lines extending from the tip of each lobe. Ribbon-shaped mesophase-pitch fibres have also been produced, obtaining a line-origin transversal texture which enhances their transport properties [6]. Recent studies demonstrated the possibility to manufacture X-type fibres which theoretically can increase ≈3–8 times the fracture energy of cementitious composites when compared to standard circular fibres [7].

Hollow carbon fibres can be fabricated by several methods such as coaxial electro-spinning, bi-polymer blends or fibre templates. A 60% hollow carbon fibre embedded in an epoxy matrix ($V_f \approx 40\%$) can result in a composite material with a density as low as 850 kg/m^3 as compared with the 1600 kg/m^3 of the standard fully dense non-hollow composite [3] demonstrating the high potential for structural lightweighting. The fibre manufacturer Toray developed hollow carbon fibres with tensile strength and modulus of 2.2 and 190 GPa, respectively, by carbonizing bi-component wet spun sheath-core fibres, with PAN as the sheath and PVA (polyvinil alcohol) as the core [3].

Circular, hollow and C-shaped carbon fibres were also manufactured by melt-spun of isotropic pitch [8–10]. Composite materials were produced by hot-press consolidation of prepregs prepared with this set of non-circular fibres by drum winding. Interlaminar shear strength specimens (ILSS) demonstrated that C-shaped CFRP's perform better as compared with circular base line composites manufactured maintaining the same equivalent cross section (the C-shape resin contact area was 2.72 times larger that the circular cross section with the same area [9]). In addition, C-shaped carbon fibre composites exhibited excellent energy absorption under impact as well as better fibre wettability and thermal conductivity than round fibres [9,10]. Patterned carbon fibres with customized surface contours were produced by [3,11] using a combination of a bi-component fibre melt spinning and a sulphonation with polyethylene (PE) precursors. By properly designing the flow path and spinneret geometry, carbon fibres with trilobal, flower, and gear-shaped cross-sections in the diameter range from 0.5 to 20 μm have been produced. Although carbon fibres produced by this method have not reached yet standard mechanical properties (tensile strength 1.1 GPa and modulus 103 GPa), the customized fibre geometry may extend their application in different fields.

Manufacturing of structural composites with non-circular fibres is still kept at laboratory scale limited by the scalability of the production process as compared with conventional circular fibres. Therefore, material optimization to achieve tailored properties based on trial and error campaigns will not be suitable at this scale and a more efficient strategy based on virtual material design and Integrated Computational Materials Engineering (ICME) can be adopted instead, at least during the first stages of the evaluation process [12]. Moreover, isolation of the effects of the fibre cross section on the composite performance may not be possible as the interface and matrix properties may be affected by the fibre shape during the manufacturing process. Computational micromechanics is emerging in recent years as a powerful tool to predict the influence of the constituent properties and the fibre shape on the ply behaviour under different loading conditions. This approach is based on the numerical simulation of the mechanical response of a *representative volume element* (RVE) of the composite microstructure [1,13–15] by means of the finite element method. As a result, this numerical strategy considers detailed information of the microstructure and constituent properties, inherited from micromechanical characterization of the fibres [16,17], matrix [18] and interface [19,20]. Computational micromechanics is used in this work to ascertain the effect of the shape of reinforcing fibres on the transverse tension and compression strength in carbon/epoxy unidirectional plies of 50% fibre volume fraction.

2. Computational micromechanics

The micromechanical model developed is based on the analysis of a representative volume element (RVE) containing a periodic and random dispersion of parallel fibres embedded in a polymer matrix representing the transversal section of an unidirectional composite ply [1,13,14]. In this work, the volume fraction of fibre reinforcement was set to 50% in all simulations, a value that is usually attained in manufacturing of common structural FRP's. No attempt to ascertain the influence of fibre volume fraction on the transverse strength properties was done in this paper although damage triggering mechanisms by debonding/matrix shear yielding should not be strongly affected in this case.

The RVE dimensions were large enough to ensure simulation results were size independent in a statistical sense, without exceeding the computational resources, to allow fast and efficient computations. A RVE of $L_0 = 58$ μm in length was enough to capture the fundamental fracture mechanisms under transverse tension (interface failure) and compression (matrix shear yielding) assuming an average diameter of the fibres of $d_f = 7.19$ μm (representative of AS4 carbon fibres). Therefore, a minimum of 8 fibres along each of the axis of the plane of transverse isotropy ($L_0/d_f \geqslant 8$) are distributed (a total of 42 in the RVE), Fig. 1. The RVE was extruded along the fibre axis with a thickness of 0.5 μm. The results were compared with RVE's containing 80 fibres to ensure that the size of the RVE did not influence significantly the model predictions.

2.1. Boundary conditions

Periodicity of the mechanical fields is guaranteed through the application of the corresponding periodic boundary conditions (PBC). PBC are imposed between opposite faces of the RVE to ensure the continuity with the neighbour RVE's as a jigsaw puzzle. For a given RVE with dimensions of $w_0 \times L_0 \times L_0$, the periodic boundary conditions are imposed as nodal displacements relations between opposite RVE faces using the following constraint equations:

$$\vec{u}(0, X_2, X_3) - \vec{u}(w_0, X_2, X_3) = \overrightarrow{U_1} \tag{1}$$

$$\vec{u}(X_1, 0, X_3) - \vec{u}(X_1, L_0, X_3) = \overrightarrow{U_2} \tag{2}$$

$$\vec{u}(X_1, X_2, 0) - \vec{u}(X_1, X_2, L_0) = \overrightarrow{U_3} \tag{3}$$

where X_1, X_2, X_3 are the coordinates axis ($0 < X_1 < w_0, 0 < X_2 < L_0, 0 < X_3 < L_0$) and $\overrightarrow{U_i}$ is the displacement of the master node i (with $i = 1, 2, 3$). As a result, three master nodes are defined on the three dimensional unit cell: $\mathrm{MN}_1(w_0, 0, 0)$, $\mathrm{MN}_2(0, L_0, 0)$, $\mathrm{MN}_3(0, 0, L_0)$. Uniaxial tension and compression in both transverse directions (X_2 and X_3) can be imposed to the RVE by applying the appropriate displacements to the master nodes. For instance, uniaxial tension or compression along the X_2 direction is imposed with $\overrightarrow{U_2} = (0, \pm\delta_2, 0), \overrightarrow{U_1} = (u_1, 0, 0)$ and $\overrightarrow{U_3} = (0, 0, u_3)$, where δ_2 (Fig. 1) stands for the tensile displacement applied, and u_1 and u_3 the lateral Poisson contractions obtained under the surface integral of the traction vector

$$\int \vec{t}\, dS = \vec{0} \text{ on } X_1 = 0 \text{ and } X_3 = 0 \tag{4}$$

Initially, a homogeneous thermal step is applied without external loading to reproduce the cooling down process from the curing (175 °C) to service temperature (15 °C). This thermal step of