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A numerical framework to analyze fracture in composite materials: From R-curves to homogenized softening laws

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ABSTRACT

A numerical framework to obtain the crack resistance curve (*R*-curve) and its corresponding softening law for fracture analysis in composite materials under small scale bridging has been developed. The use case addresses the intralaminar transverse tensile fracture of a unidirectional ply of carbon fiber-reinforced polymer AS4/8552. The *R*-curve is computed for this material using a micromechanical embedded model corresponding to the intralaminar transverse tensile fracture toughness characteristic. The model combines an embedded cell approach with the Linear Elastic Fracture Mechanics (LEFM) displacement field to analyze the local crack growth problem including fiber/matrix interface debonding and matrix ligaments bridging as the main energy dissipation mechanisms. Other large scale toughening effects as, for instance, fiber bridging were not included in the model. Parametric analysis were carried out to assess the influence of the properties of the material constituents on the *R*-curve behavior and on the corresponding homogenized cohesive laws.

1. Introduction

Polymer matrices reinforced with high performance fibers, or FRPs, are preferred candidates for structural applications driven by lightweight design and nowadays are very common in the aerospace, automotive and energy industries as well as sports and leisure goods. One of the main drawbacks limiting a wider use of these materials is the difficulty to predict their mechanical behavior under service conditions due to the complex deformation and failure mechanisms that very often lead to well-known *black metal* design guidelines. Such complexity level is experimentally revealed at different lengths scales in which a FRP material is hierarchically organized, namely the ply ($\sim 10-100$ µm), the laminate ($\sim 1-5$ mm) and the structural component (~ 1 m) (Llorca et al., 2011). For instance, at the microlevel, intralaminar failure occurs due to a competition of mechanisms, triggered by the local stress state in the ply, between matrix cracking and shear banding, fiber brittle failure as well as fiber/matrix interface debonding. At this length scale, the properties of the constituents as well as the spatial distribution play the critical role in the fracture process although defects generated from manufacturing, such as voids, interface debonds or resin pockets, may alter this situation. These intralaminar ply mechanisms are well described in the literature and have helped considerably to develop physically based computational homogenization models (Pinho et al., 2009; Canal et al., 2012). Such kind of models rely on the existence of a statistically representative volume element (RVE) whose microstructure can be generated synthetically including all relevant failure mechanisms observed in the real material (Vaughan and McCarthy, 2010). The techniques were successfully applied to predict ply strength of unidirectional plies subjected to homogeneous stress states including tension, compression, shear (González and LLorca, 2007; Totry et al., 2010), and their combinations in a failure locus (Totry et al., 2008), including the effect of environmental conditions (Naya et al., 2017). To avoid artificial damage and boundary layer effects, most of the computational homogenization models make use of periodic RVEs applying homogeneous stress states through periodic boundary conditions imposed by constraining the relative displacements of pairs of opposite nodes in the model.

The ability of computational homogenization models based on periodic RVEs rely on good idealizations of the current material microstructure as well as constitutive models of the constituents to explicitly reproduce damage onset and propagation and their continuous interaction (Segurado and Llorca, 2002). On the other hand, their major drawback is the inability to describe material softening after the occurrence of strain localization. To overcome such limitation, models including detailed descriptions of the

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microstructure of the material in the fracture process zone can be used to deal with localized crack propagation problems where material toughness determination is required. The region out of the fracture process zone in embedded models is formed by a homogenized material with equivalent properties of the overall elastic behavior of the composite. Embedded models were successfully applied in the past to simulate fracture of unidirectional plies from a micromechanical perspective including matrix plasticity, fiber bridging and pull out in Ti/SiC composites (González and LLorca, 2006; 2007) and fiber/matrix interface debonding with ductile tearing of matrix ligaments (Canal et al., 2012). However, an important problem when dealing with embedded cells is the inadequacy to represent at the same discretization level, fracture mechanisms spanning different length scales. For instance, the characteristic fracture process length for brittle epoxy matrices is $l_c \approx 20$ µm while the case of fiber toughening effects to fiber bridging crossovers is $l_c \approx 1-5$ mm (Bao and Suo, 1992). Considering these important drawbacks, embedded models can be used to infer the shape of softening laws in composite materials based on the adequate description of the individual constituents failure mechanisms and their interaction during the propagation of a crack.

In this work, a numerical methodology based on computational homogenization to analyze fracture in heterogeneous materials under *small scale bridging* (SSB) conditions is presented. Due to the complexity of the problem, the methodology is illustrated to study the bidimensional propagation of a crack in a fiber reinforced unidirectional ply, including the fiber/matrix interface debonding and the ductile tearing of the matrix ligaments between fibers as energy dissipation mechanisms. This crack propagation problem is also known as the intralaminar crack propagation under transverse tension characterized by the fracture toughness G_{2+}. The bidimensional formulation of the problem impedes the inclusion of higher length scale toughening mechanisms, as for instance, fiber bridging due to the lack of parallelism between fibers, so the material toughness and R-curve behavior obtained should be understood as lower bounds or initiation values rather than propagation over a finite crack length of some mm (Pinho et al., 2009). Homogenized softening laws for the crack propagation problem in a unidirectional ply are presented for a wide range of micromechanical parameters including constituent properties as the fiber/matrix interface and matrix plastic/damage behavior.

The paper is organized as follows. The description of the model framework is carried out in Section 2, where the embedded micromechanical model under small scale bridging and the corresponding homogeneous cohesive crack approach are described. In Section 3, the models are applied to determine the *R*-curve behavior and the energy equivalent softening laws for a baseline set of micromechanical parameters. The ability of computational micromechanics to address the influence of the micromechanical properties of the constituents is discussed in Section 4 while the final remarks and conclusions are drawn in Section 5, respectively.

2. Methodology

2.1. An embedded cell model for crack propagation

A simulation methodology was developed to infer the *R*-curve behavior and investigate softening laws based on computational micromechanics to address crack propagation problems in unidirectional fiber reinforced composites. The modeling strategy was applied to study the intralaminar transverse fracture toughness of a unidirectional UD carbon/epoxy system AS4/8552 (Herráez et al., 2015; Naya et al., 2017) using as inputs the micromechanical parameters and the reinforcement distribution. The model was only applied to study the bidimensional crack propagation assuming the matrix tearing and fiber/matrix interface debonding as the dominant energy dissipation mechanisms. The crack front is assumed to be parallel to the fiber direction, namely x_1, and running in the plane $x_2 - x_3$ as shown in Fig. 1. The model includes the microstructure of the material, but, only in a small region close to the crack tip known as fracture process zone (FPZ). This detailed region of size $\ell = 1500$ µm$\times h = 100$ µm is embedded in a larger rectangular area $L = 76,800$ µm $\times H = 19,200$ µm. This methodology allows the isolation of the crack propagation problem from any global specimen geometry effect. The microstructure used for the embedded region corresponds to a homogeneous dispersion of parallel fibers aligned in the x_1 direction, being the fiber volume fraction $V_f = 65\%$, Fig. 1. A typical embedded model contains over 2400 fibers with diameter 7.2 ± 0.2 µm, representative of AS4 carbon fiber (Naya et al., 2017; Herráez et al., 2015). The rest of the model, out of the embedded region, was treated as a homogeneous transversely isotropic elastic solid whose behavior is given by any suitable homogenization scheme from the elastic constants of the constituents, fibers and matrix, and the volume fraction of reinforcement. The two regions of the model share the bounding nodes, so the displacement continuity is guaranteed. The width of the embedded model, $h = 100$ µm, was large enough to ensure the effect of the transition from heterogeneous to homogeneous solids induced negligible effects in the crack propagation process. The mesh size was set to ≈ 1 µm in the embedded region and it progressively grows along the homogeneous region up to ≈ 480 µm at the outer edges. This discretization level ensures good representation of stress fields at the microlevel while maintaining acceptable computation times. A typical baseline model is formed by 385,000 elements. Simulations were carried out using the implicit dynamic solver in Abaqus/Standard, the quasi-static solution settings and within the framework of the finite deformations theory with the initial unstressed state as the reference one.

Table 1
Elastic properties of the AS4 carbon fibers (Herráez et al., 2015; 2016), 8552 epoxy matrix (Rodríguez et al., 2012b; Naya et al., 2017) and the composite through RVE computational homogenization with ($V_f = 65\%$) (Naya et al., 2017).

Material	E_1 (GPa)	E_2 (GPa)	ν_{12}	ν_{23}	G_{12} (GPa)	G_{23} (GPa)	ρ (kg/m^3)
Fibre	231.6	12.97	0.3	0.46	11.3	4.45	1780
Matrix	5.07	–	0.35	–	–	–	1260
Composite	152.3	7.17	0.32	0.48	4.1	2.42	1600

The whole model was discretized using a lagrangian mesh with finite elements. The matrix, fibers and the homogenized region were modeled with 4-node fully integrated quadrilateral isoparametric plane strain elements (CPE4) in Abaqus/Standard (Simulia, 2013). The fiber-matrix interface debonding was simulated with 4-node cohesive isoparametric elements (COH2D4) inserted at each of the individual fiber/matrix interfaces (Camanho and Davila, 2002; Turon et al., 2006).

Fibers were modeled as linear elastic transversely isotropic solids representative of a typical carbon fiber used in unidirectional reinforcements. Their elastic constants are reported in Table 1. The elastic properties corresponding to the homogenized medium out of the embedded region for $V_f = 65\%$ volume fraction were determined by computational homogenization using FEM analysis of periodic representative volume element models in the elastic regime (Naya et al., 2017) and the results are included in Table 1.

The polymer matrix behavior is represented using a damaged/plasticity model originally developed by Lubliner et al. (1989), which is included in Abaqus/Standard (Simulia, 2013) that accounts for both, plastic yield under compressive/shear loads as well as brittle failure due to dominant tensile stresses. Under uniaxial tensile stress, the matrix exhibits linear softening once the tensile strength is reached, σ_{t0}. The energy dissipated by the matrix

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