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In-depth numerical analysis of the TDCB specimen for characterization of self-healing polymers

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ABSTRACT

The Tapered Double Cantilever Beam (TDCB) is the common specimen to study self-healing thermosetting polymers. While this geometry allows characterising the mode I fracture toughness without taking into account the crack length, the experiments show an important dispersion and unstable behaviour that must be taken into account to obtain accurate results. In this paper, finite element simulations have been used to understand the experimental behaviour. Static simulations with a stationary crack give the local stresses and the stress intensity factors at the crack tip when the TDCB is under load. In addition, the eXtended Finite Element Method (XFEM) has been used to make quasi-static crack propagation simulations. The results indicate that the crack tip has a curved profile during the propagation, advancing more at the edges than at the centre. The crack propagation begins when the applied load reaches a critical value. The unstable crack propagation noted in the experiments can be reproduced by introducing an unstable behaviour in the simulations. Finally, the sensitivity of the critical load has been studied as a function of the friction between pin and hole, tolerance of geometrical dimensions, and cracks out of the symmetric plane. The results can partially explain the dispersion of the experimental data.

1. Introduction

Self-healing polymers have the additional ability of recovering the structural properties with or without external aid (White et al., 2001). This ability is an advantage for structural polymers that are susceptible to suffer mechanical degradation due to damage in form of cracks. Self-healing polymers open a window to new structural materials such as self-healing composites. The study of self-healing polymers is the first step to approach such self-healing composites.

There are several self-healing concepts for polymers (Billiet et al., 2013; Yuan et al., 2008b) . On the one hand, there are intrinsic self-healing polymers based on a matrix that can repair damage due to cracks by itself under a certain stimulation (Jud et al., 1981; Jud and Kausch, 1979; Meure et al., 2009; Raghavan and Wool, 1999), mostly heating. Currently, most of these self-healing polymers cannot heal themselves without an external intervention. On the other hand, there are extrinsic self-healing polymers that have a healing agent embedded or encapsulated which is responsible for the repair (Toohey et al., 2007; White et al., 2001). The healing agent can be embedded into tubes making a vascular network or encapsulated in capsules. The size of these tubes or capsules can be of the order of microns. When the cracks break the tubes or capsules, the healing agent is released in the crack plane. In this case, the self-healing polymer usually does not need an external aid to repair the damage because there is a chemical trigger in the system. Consequently, the released healing agent in the crack plane is polymerized when coming into contact with the chemical trigger, and the structural integrity across the crack plane is re-established. They can be considered autonomous self-healing polymers.

This study deals with autonomous micro-encapsulated polymers. In these systems, the liquid healing agent is encapsulated in microcapsules which are dispersed in the polymer, and the chemical trigger can be found in solid state embedded inside the matrix (Blaiszik et al., 2008; Brown et al., 2002, 2005; White et al., 2001), or in liquid state encapsulated in a second sort of

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microcapsules (Yuan et al., 2008a, 2009). This second system with two types of microcapsules makes it possible to use a huge amount of click reactions in the design of self-healing polymers (Billiet et al., 2012; Hillewaere et al., 2014).

The studies about micro-encapsulated self-healing polymers evaluate self-repair by comparison of the final mechanical properties of the healed polymer and the initial properties of the virgin one (Wool, 1981). The most common value to quantify the self-healing performance is the ratio between the healed and virgin fracture toughness. Therefore, healing efficiency is defined as $\eta = K_{IC}^{healed}/K_{IC}^{virgin}$ (White et al., 2001). Several works employ a Tapered Double Cantilever Beam (TDCB) fracture geometry to simplify the measurement of the healing efficiency (Brown, 2011; Rule et al., 2007; Brown et al., 2002, 2004, 2005). In the TDCB geometry, the fracture toughness is independent of the crack length a and proportional to the critical load P_C (Mostovoy et al., 1967), which triggers the crack growth. Then, the fracture toughness can be written as $K_{IC} = \alpha \cdot P_C$, where α is a constant obtained from the geometry and the material properties, and the healing efficiency is determined by the ratio of the critical loads, $\eta = P_C^{healed}/P_C^{virgin}$.

The TDCB geometry, adapted to simplify the study of self-healing polymers, is useful to obtain the healing efficiency, but several details must be taken into account to obtain accurate values. In addition, the limited fracture information extracted from the TDCB highlights the demand for other experimental geometries that may complete the characterization of the self-healing polymers. An accurate value of the fracture toughness and fracture energy can be obtained from the compact tension fracture test for plastic materials (ASTM Standard D 5045). In addition, tensile properties, such as Young's modulus, Poisson's ratio, yield strength and ultimate tensile strength, can be measured from the tensile test for plastic materials (ASTM Standard D 638).

The current paper focuses on the response of the TDCB specimen applied to study the healing performance of micro-encapsulated thermosetting polymers. We use the Finite Element Method (FEM) combined with recent techniques to follow the crack propagation based on eXtended Finite Element Method (XFEM). The commercial software ABAQUS has implemented this methodology. Simulations show in detail how the mechanical failure is produced in the TDCB experiments, giving information about the critical force, crack profile and the local stress intensity factor. First, we describe the TDCB specimen and the model in detail. Then, the results from the simulations are explained and compared with experimental values. Finally, the effect of the geometry dimensions and boundary conditions has been studied.

2. TDCB specimen

2.1. Geometry

Although the TDCB geometry is described in several papers, we have taken the dimensions used by Brown et al. for samples with EPON 828 (Brown, 2011; Brown et al., 2002, 2004). Fig. 1(a) shows the geometry and the dimensions in millimetres. We have fixed the radius of the pin holes to 6 mm and the radius of the fillet edges to 2 mm. This geometry fits White's protocol (White et al., 2001) to determine the healing efficiency.

The TDCB geometry is defined by the thickness b and the height profile $h(a)$. The height profile of the geometry is designed so that the mode I fracture toughness K_I is constant in the range of the crack length a between 20 and 40 mm (Brown, 2011). Therefore, K_I is linear with the load applied between the pins. This is possible because the change in compliance with respect to the crack length remains constant (Mostovoy et al., 1967). The differences between TDCB and other geometries have been fully discussed by Brown (2011). The crack propagation behaviour with constant compliance is shown in the experiments and it can be reproduced with the simulation as we show in the next section.

It is important to notice that two grooves along the horizontal plane xOz were added to prevent the crack from changing its direction. The final thickness of the crack plane b_n is lower than the thickness of the sample b (see the detail of grooves in Fig. 1(b)). In order to define the geometry of the grooves, we have fixed an angle of 45° for the side grooves and the two thicknesses, b and b_n.

We have included an extra dimension in the geometry of the TDCB that has been neglected in previous works (Brown, 2011; Brown et al., 2004; White et al., 2001). This is a small height, d_n, in the horizontal plane (Fig. 1(b)). One reason to introduce this dimension is that the real TDCB specimen always has a rounded end in the side of the grooves. Modelling these edges with a certain height d_n is more realistic than a sharp geometry. In addition from the numerical point of view, the height d_n is twofold: allows us to discretize the volume more easily and prevents numerical singularities.

It is needed to define a pre-crack in the geometry of the TDCB specimen to complete White's protocol. The pre-crack is located in the horizontal plane xOz with a length between 2 to 5 mm. In the experiments the pre-crack is performed by manually tapping with a razor. We have observed that the experimental results are strongly dependent on the performed pre-crack (Tsangouri et al., submitted for publication). In Section 5, we will discuss this issue and its sensitivity.

2.2. Material properties

In the present work we have used the epoxy EPON 828. This epoxy is well known in the aerospace industry and is fully characterised in the reference (Brown et al., 2004). It is noteworthy that EPON 828 has been used in several studies of self-healing polymers with micro-capsules (Brown et al., 2002, 2004, 2005, 2006; White et al., 2001). The EPON 828 resin and the diethylenetri-amine (DETA) hardener are mixed in equimolar distribution (100/11 w/w ratio epoxy/hardener). The usual curing program is 24 h at room temperature and 24 h at 40 °C (Billiet et al., 2013). In this work we will consider EPON 828 as brittle material without plastic behaviour (see properties in Table 1). Because of the brittle behaviour of the polymer, we assume that the yield strength and the ultimate tensile strength are equal, $\sigma_Y = \sigma_{UT}$.

In addition to the epoxy properties, we have included the first order radius of the plastic zone around the crack tip, obtained from

$$r_\rho = \frac{1}{2\pi}\left(\frac{K_{IC}}{\sigma_Y}\right)^2 \tag{1}$$

where K_{IC} is the mode I fracture toughness and σ_Y the yield strength. r_ρ has been used to find the correct size of the mesh elements along the crack plane and it is further discussed in the next section with the results of the model.

2.3. Experimental setup

The setup of the experiment with the TDCB specimen is described in references (Brown et al., 2002, 2004). The specimen is supported by two pins inside each hole. Each pin allows free rotation along its rotational axis. During the experiment, a constant vertical displacement is applied in the upper pin while the lower pin is fixed. As a result, the crack propagates along the horizontal plane defined by the grooves. The reaction force and displacement in the upper pin are recorded during the experiment to obtain load–displacement curves. Then, the critical load P_C can be obtained from the curves.