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3D study of the competitions between shear yielding and crazing for a variable thickness on ductile polymers

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ABSTRACT

The influence of the thickness in mode I fracture tests is investigated with extensive 3D finite elements calculations. A realistic constitutive law for the bulk is used. Failure by crazing is described with a cohesive model. A transition from ductile tearing to fracture by crazing is observed with increasing thickness. Ductile tearing takes place for thin samples even if possible crazing is allowed. Crazing takes place for thick samples with a noticeable difference in the load level for craze initiation to that for crack propagation. The consequence on the appropriate geometry for the estimation of the minimum toughness is discussed.

1. Introduction

Failure characteristics and toughness estimations of the toughness at the onset of crack propagation are investigated. Polycarbonate is taken as representative of a ductile glassy polymer at room temperature, but also because of its commercial importance in structural application. Its fracture toughness is known to be dependent on a number of factors including the molecular weight, the processing, including ageing time, loading rate and specimen geometry. In the present paper, the influence of the specimen geometry is investigated and in particular that of the thickness, which is the only varied parameter. For thick specimen, fracture in glassy polymers depends on the competition between shear yielding and crazing, which are two rate dependent plastic mechanisms, although at different length scales. Shear yielding corresponds to strain localization in the form of shear bands related to the bulk constitutive law with softening upon yielding followed by hardening at continued deformation. Crazing involves also some plasticity but at the micron scale. A rate dependent description of these two mechanisms is accounted for by Estevez et al. [14] who showed that the ductile to brittle transition with increasing loading rate can be captured and is related to a reduction in the bulk plasticity prior to failure. Their analysis is performed under the assumption of 2D plane strain conditions which imply an infinitely large thickness. The influence of the specimen thickness is investigated here for a given polycarbonate in terms of molecular weight, processing and ageing time. A unique geometry corresponding to a single edge notch specimen (SENT) subjected to uniaxial tension is considered with a blunt notch R of 0.25 mm. A blunt notch is accounted for as sharp cracks are difficult to machine in PC. It allows for a well defined geometry. The thickness t is varied from $t/R = 1$ to 16, larger ratios being considered in some cases. Evidences of the influence of the

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thickness on the fracture toughness are reported by Parvin and Williams [34], Fraser and Ward [18] for instance, while Nisitani and Hyakutake [32] investigated the influence of the notch radius. The toughness is observed to decrease with increasing thickness and in the present study, we use the ratio t/R to characterize the 3D effects, with a fixed notch radius R and variable thickness t.

The ductile to brittle transition in ductile polymers is not only related to loading rate effects governed by the time scales between the test rate and those involved in shear yielding and crazing. For a given test condition in terms of loading rate, increasing the thickness from thin or film samples to thick specimens results in two fracture modes: ductile tearing in the case of polymer films and thin samples to failure by crazing for thicker ones [34]. For thin samples, a flame like plastic zone is observed ahead the notch tip [22,10] and failure takes place by ductile tearing for a critical cumulated plasticity [20,21]. For thick samples, the shape of the plastic zone is similar to slip lines predicted by Hill [23] with localized plasticity in the form of shear bands [28]. In ductile polymers, failure by crazing is generally preceded by the development of this latter type of plastic zone with the initiation of crazing at the tip of the plastically deformed region [24,31]. In the literature, a criterion for the onset of failure is associated with the initiation of crazing [28,20,21,5,27] and a single critical mean stress is usually considered sufficient to predict the onset of failure. The estimation of the critical stress state for craze initiation is derived from 2D plane strain calculations [24,31]. A value ranging in 70–90 MPa is found. The estimation of the critical stress state for the nucleation of crazing requires a 3D analysis as the stress distribution around the notch is noticeably thickness dependent so that a condition derived from 2D plain strain calculation results is an upper bound for its estimation. The appropriate criterion for craze initiation remains an open question in the polymer community as illustrated in the numerous expression found in the literature [37,33,3,24,36,8,17] based on experimental observations, continuum models or molecular dynamics calculations: criteria based on a critical mean stress or combining the shear and mean stress or simply the maximum principle stress are found.

Craze thickening ensures some load carrying capacity so that failure corresponding to craze fibrils breakdown takes place for a load level larger that can be larger to that for craze initiation. The description of the mechanism underlying failure, even in a simplistic form appears more suitable to estimate the fracture toughness.

The objective of this work is to gain insight on the estimation on whether plane stress and/or plane strain conditions are dominant or combined in the characterization of glassy polymer fracture, under quasi-static conditions. A numerical study is carried out with the implementation of Boyce et al. constitutive law [7] in the version modified by Wu and Van der Giessen [41] to realistically capture the stress–strain fields around the notch. The Single Edge Notched Tension (SENT) configuration is considered with a given dimension regarding the height, width and crack length. A configuration with a blunt notch specimen is preferred to that with a natural crack as experimentally machining a natural crack is difficult in ductile polymers while preparing a blunted one is tractable. 3D effect on glassy polymer fracture have been investigated recently by Gearing and Anand [21] and Kattekola et al. [27] for a given thickness [21] and variable thickness [27]. In these studies, failure is considered when a continuum criterion is met first: a critical plastic stretch or a critical mean stress, depending on the stress triaxiality of the test [21] or on the specimen thickness [27]. In the present study, a simple cohesive model is used to mimic crazing mechanically with a traction separation law of which maximum traction and critical opening are representative for crazing that appears as an extension of these investigations. The influence of the specimen thickness on the fracture toughness is investigated first for a set of reference material parameters, representative of polycarbonate for the bulk. The maximum traction for triggering cohesive debonding is adjusted to allow prior development of plasticity as observed in ductile polymers. The influence of the softening upon yielding is investigated first and next that of the cohesive critical opening (and related energy of separation) is explored. In both cases, the variation of the predicted toughness with the thickness is reported. Comments on the appropriate thickness to derive a minimum toughness are eventually provided, which are thought useful for practical applications.

The present paper is organized as follows: the governing equations for the bulk constitutive law are presented with the adopted bulk parameters followed by a presentation of the cohesive model for failure. The problem formulation is presented and the simulations results presented. A discussion and conclusive remarks complete the paper.

Tensors are denoted by bold face symbols, $\otimes$ is the product tensor and $\bullet$ the scalar product. For example, with respect to a Cartesian basis $\boldsymbol{e_i}$, $\boldsymbol{AB} = A_{ik}B_{kj}\,\boldsymbol{e}_i \otimes \boldsymbol{e}_j$, $\boldsymbol{A} \bullet \boldsymbol{B} = A_{ij}B_{ij}$ and $\mathbb{L}\boldsymbol{B} = \mathbb{L}_{ijkl}B_{kl}\,\boldsymbol{e}_i \otimes \boldsymbol{e}_j$, with summation implied over repeated Latin indices. The summation convention is not used for repeated Greek indices. A prime $(\ )'$ identifies the deviatoric part of a second-order tensor, $\boldsymbol{I}$ the second identity tensor and tr denotes the trace.

2. Constitutive law for glassy polymers

We present the governing equations of the constitutive model used to capture realistically de stress–strain fields of glassy polymers and then the set of parameters used in the study.

2.1. Modelling background

The constitutive law used to model the large strain plasticity is based on original ideas due to Boyce et al. [7] but with some modifications introduced later by Wu and Van der Giessen [40] for the hardening part. The constitutive equations pre-