Journal of the Mechanics and Physics of Solids 93 (2016) 182–197

Contents lists available at ScienceDirect

Journal of the Mechanics and Physics of Solids

journal homepage: www.elsevier.com/locate/jmps

Phase field modeling of damage in glassy polymers

Yuesong Xie [a], Oleksandr G. Kravchenko [b], R. Byron Pipes [b], Marisol Koslowski [a,*]

[a] *School of Mechanical Engineering, Purdue University, West Lafayette, IN 47907, United States*
[b] *School of Aeronautics and Astronautics, Purdue University, West Lafayette, IN 47907, United States*

ARTICLE INFO

Article history:
Received 27 July 2015
Received in revised form
6 November 2015
Accepted 30 December 2015
Available online 19 January 2016

Keywords:
Phase field
Fracture
Polymers

ABSTRACT

Failure mechanisms in amorphous polymers are usually separated into two types, shear yielding and crazing due to the differences in the yield surface. Experiments show that the yield surface follows a pressure modified von Mises relation for shear yielding but this relation does not hold during crazing failure. In the past different yield conditions were used to represent each type of failure. Here, we show that the same damage model can be used to study failure under shear yielding and crazing conditions. The simulations show that different yield surfaces are obtained for craze and shear yielding if the microstructure is included explicitly in the simulations. In particular the breakdown of the pressure modified von Mises relation during crazing can be related to the presence of voids and other defects in the sample.

1. Introduction

Extensive experimental evidence shows that failure of glassy polymers is influenced by deviatoric and volumetric components of deformation. Due to this claim the most widely used yield criterion is a pressure-modified von Mises condition of the form:

$$\sigma^{dev} = \sigma_{crit} - \mu_{vM}\sigma^{vol} \tag{1}$$

where σ_{crit} is a constant representing the stress required for yielding under pure shear stress and μ_{vM} is a coefficient that describes the dependence of the deviatoric stress on the volumetric stress at failure. This coefficient is temperature dependent and it is in the range 0.3–1 (Quinson et al., 1997). The volumetric stress and deviatoric stress in Eq. (1) can be written in terms of the principal stresses as

$$\sigma^{vol} = \frac{\sigma_{11} + \sigma_{22} + \sigma_{33}}{3} \tag{2}$$

$$\sigma^{dev} = \sqrt{\frac{1}{2}\left[(\sigma_{11} - \sigma_{22})^2 + (\sigma_{22} - \sigma_{33})^2 + (\sigma_{33} - \sigma_{11})^2 \right]} \tag{3}$$

Fig. 1 shows yield surfaces for polymethyl methacrylate (PMMA) from the experimental work of Quinson et al. (1997) and Bowden and Jukes (1968). Quinson et al. (1997) tested three different loading conditions at room temperature: uniaxial compression, plane strain compression and simple shear. The onset of yielding is determined by these authors when the

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[*] Corresponding author.
E-mail address: marisol@purdue.edu (M. Koslowski).

http://dx.doi.org/10.1016/j.jmps.2015.12.021
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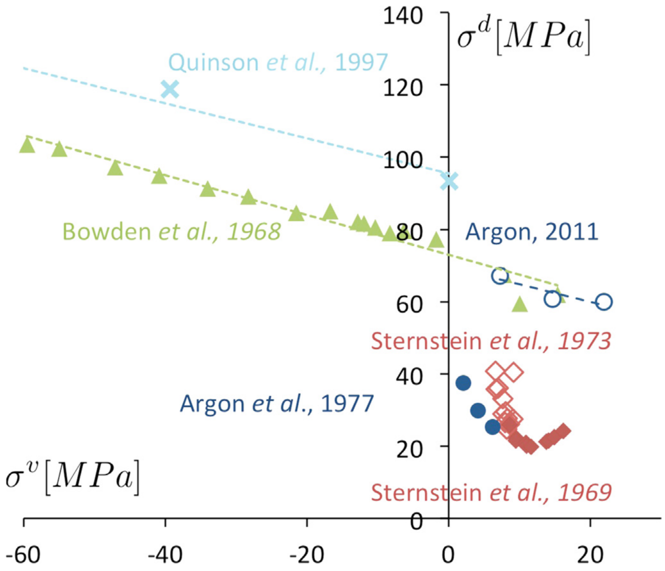

Fig. 1. Yield surfaces for PMMA extracted from the experiments of Quinson et al. (1997) (blue crosses), Bowden and Jukes (1968) (green triangles), Sternstein and Ongchin (1969) (solid red diamonds), Sternstein and Myers (1973) (open red diamonds), and for polystyrene from the experiments of Argon and Hannoosh (1977) (solid blue circles) and Argon (2011) (open blue circles). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

maximum loading stress with zero residual strain is reached. Bowden and Jukes (1968) investigated plane strain compression of thin sheets of PMMA at room temperature. The yield condition in this case is determined at the maximum compressive stress. These yield surfaces correspond to shear and compressive stresses conditions and follow the pressure-modified von Mises condition in Eq. (1).

The experiments of Sternstein and Myers (1973), Argon and Hannoosh (1977) and Argon (2011) examined the behavior under tensile loading. Under this condition zones of fibrillation or crazes develop that result in brittle failure of the polymer. The onset of crazing observed in these experiments is also shown in Fig. 1. The data of Sternstein and Ongchin (1969) is obtained for PMMA and the experiment of Argon and Hannoosh (1977) is for polystyrene. The results of Argon and Hannoosh (1977), correspond to the applied stress at the onset of crazing while in a later work Argon (2011) calculated the local values of stress from a model that takes into account initial surface grooves. It is clear that under positive volumetric stress the yield surface in some experiments do not follow Eq. (1).

Due to its engineering impact, polymer damage has been the focus of extensive modeling efforts. A number of computational models, ranging from atomistic (Mahajan and Hartmaier, 2012; Jaramillo et al., 2012) to continuum (Estevez et al., 2000; Tijssens et al., 2000; Seelig and Van der Giessen, 2009; Ponson and Bonamy, 2010; Heyden et al., 2015), have been utilized to study polymer failure as well as polymer composite materials (Totry et al., 2008; Mendoza-Jasso et al., 2011; Tran et al., 2012). While atomistic simulations give insight information into the material behavior, a connection to experimental results remains elusive due to the differences in time and length scales. At the continuum level new mathematical approaches to failure are being developed in which the damage is characterized by a single material parameter that can be calibrated with experiments or atomistic simulations. In these theories a phase field variable indicates how damage is extended over the domain and its evolution (Francfort and Marigo, 1998; Amor et al., 2009; Miehe et al., 2010; Pandolfi and Ortiz, 2012; Hesch and Weinberg, 2014). A difference with previous approaches such as cohesive zone models is that the damage is not limited to a two dimensional manifold but it is defined over a finite volume which makes the phase field method advantageous for crazing and shear yielding where diffuse damage zones are observed (Quinson et al., 1997).

In this paper, numerical simulations with a phase field damage model (PFDM) are performed to study the onset of yielding in amorphous polymers. Two different brittle damage models that separate volumetric and deviatoric contributions are considered in the PFDM. In the first model, introduced by Amor et al. (2009), only the dilatational and the deviatoric part produce damage. The second model, developed by Miehe et al. (2010), takes into account the sign of the principal strain directions. The predicted yield surfaces show that to obtain hardening in compression it is necessary to consider the sign of the individual principal strain directions and therefore, the second model is adopted. The parameters of this model are calibrated with experiments performed in a simple tension dog bone and a single edge notch tension (SENT) PMMA specimen. The calibrated model is used to reproduce the loading conditions in the experiments in Fig. 1. The simulations show that the same PFDM model can be used to predict the experimental results in Fig. 1. Including voids in the sample explains the difference in the behavior under positive volumetric stress during the onset of crazing.

The paper is organized as follows, in Section 2 the PFDM is presented. The PFDM is calibrated against two experiments in Section 3. The calibrated model is used to predict the behavior of PMMA in different loading conditions and geometries. A summary of the results is in Section 4.