Influence of damage on inhomogeneous deformation behavior of amorphous glassy polymers. Modeling and algorithmic implementation in a finite element setting

Sami Holopainen

Tampere University of Technology, Department of Engineering Design, P.O. Box 589, 33 101 Tampere, Finland

ARTICLE INFO

ABSTRACT

The objective of this work is to investigate the influence of damage mechanisms on inhomogeneous deformation behavior of amorphous glassy polymers. The mechanical properties of glassy polymers are strongly influenced by the microstructure which is typically described by network models. In order to improve the network model predictions at large multidimensional deformations, a distributed growth of void volume, crazing and possible disentanglement are investigated and considered in a part of the proposed viscoelastic–plastic model. The importance of different rheological properties employed in the model for regarding mechanical behavior is investigated and the role of damage in localized deformation is addressed. In order to evaluate the predictions of the proposed model, algorithmic constitutive equations are derived and implemented in a finite element program. The model is employed to the simulation of the cold drawing of dumbbell shaped test specimen.

© 2014 Elsevier Ltd. All rights reserved.

Nomenclature

- Mechanics of materials.
  - Constitutive modeling of amorphous glassy polymers.
    - Modeling of inhomogeneous deformation behavior.
      - Plasticity, shear bands.

    - Modeling of damage mechanisms.
      - Void growth, crazing, disentanglement.
      - Evaluation of possible void coalescence.

  - Algorithmic treatment and finite element method.

1. Introduction

It is widely acknowledged that the macroscopic mechanical behavior of amorphous glassy polymers stems from three major microstructural characteristics: the number of entanglements and statistical links between the entanglements, the

E-mail address: Sami.Holopainen@tut.fi

growth of shear bands and the extent of free volume around the chain molecules, cf. e.g. [1–4]. Moreover, amorphous glassy polymers exhibit several damage processes such as crazing, cavitation of impurities and micro-cracking within the matrix material. Onset of the volume changes in amorphous glassy polymers are the growth and coalescence of existing voids in addition to the nucleation and growth of new voids. Under compression, amorphous polymers frequently show ductile localized deformation, which is due to shear yielding with small volume changes. In contrast to the shear yielding mechanism, which involves shear band propagation and eventual fracture by a chain scission in large strains, the governing mechanism of inelastic deformation under tension is a dilatational localization in zones of fibrillation, termed crazing, cf. [5,6].

Ref. [7] conducted plane strain compression tests both on polymethylmethacrylate (PMMA) and on polystyrene (PS) to investigate the formation of shear bands. According to their observations, the growth of shear bands is the primary source for the evolution of plastic deformation in amorphous glassy polymers. The plane strain tension tests by [8] showed a remarkable drop in the macroscopic stress immediately after the development of macroscopic shear bands. During continued deformation, the propagation of shear bands and the development of inhomogeneous deformation were observed which is macroscopically manifested by necking.

Ref. [9] investigated the influence of damage (crazing, cavitation of rubber particles and micro-cracking within the matrix material) on the plastic deformation and stability in polyethylene terephthalate (PET) and high-impact polystyrene (HIPS). Based on the optical micrographs, shear bands nucleated from the tips of existing crazes, rather than the crazes being nucleated at the intersection of fine shear bands. They concluded that the onset of plastic deformation is initiation of crazing and the plastic stability is essentially controlled by damage processes such as craze-widening. To trigger a transition from crazing to shear yielding, some heterogeneity, which relieves the build-up of high hydrostatic stress, is needed in the amorphous structure, cf. [10]. In contrast to tensile tests, where the initial chain distribution have been found to be macroscopically uniform, large-scale molecular dynamics (MD) simulations have indicated that the chain distribution locally is heterogeneous, cf. [11]. As a result of heterogeneity, polymer material shows localized deformation where microscopic shear bands in closely packed regions develop and annihilate into macroscopic shear bands. Ref. [11] also showed that the thickness of the ligaments within the structure is crucial.

Despite all the active research carried out during the last decades, the governing micromechanism that controls crazing is still not fully understood. Experimental investigations have shown a major importance of the entanglement density in macroscopic failure through crazing or shear yielding, cf. e.g. [10,12–14]. Initial plastic deformation through shear yielding in amorphous glassy polymers is usually followed by crazing or alternatively crazing propagates on stable manner, cf. [9,15]. Examples of the polymers in the first group are e.g. polycarbonate (PC) and PMMA, and polymers involving stable crazing are e.g. HIPS and polyacrylonitrile–butadiene–styrene (ABS) that are frequently used in toughened polymer blends. According to [15], decrease of temperature and increase of the strain rate result in more brittle failure in amorphous glassy polymers, i.e. the difference between the time instants for craze-initiation and breakdown decreases. They also pointed out that the void nucleation is a precursor to crazing and crazes initiate due to high mean stress concentrations around the micro-voids. As a result of the damage processes, volume strains in relation to total strains, i.e. the plastic dilatation, was found to be significant. Ref. [16] conducted molecular dynamic MD simulations to investigate the role of deformation-induced disentanglement to void nucleation in amorphous glassy polymers. They concluded that disentanglement increases under highly triaxial stress states, which results in void nucleation being increased. They also pointed out that porous regions are created at the locations where almost all the polymer chains have slipped away except a few that are firmly anchored at their ends and pulled taut.

Most of the current models are based on the assumption that the plastic deformation only evolves because of the development and propagation of shear bands without volume changes. Concerning void growth, many of the inelastic damage models available for amorphous glassy polymers are based on the explicit knowledge of the yield surface involving a large number of material parameters to be identified, cf. [17–21]. However, the damage processes observed in amorphous glassy polymers are complex phenomena and their modeling seems to require such complexity. The models developed for metals have initially been considered for that purpose, cf. e.g. [22,23]. Based on plane strain finite element simulations [24] investigated the effects of pressure sensitive yielding and plastic dilatancy on void growth and void mutual interaction. They concluded that void growth is promoted by pressure resulting higher porosity and void interaction in the material during loading. A widely used dilatational plasticity model is the one introduced by [25] and later modified by [26]. The Gurson model is based on the assumption that the deformation mode of the material surrounding a void is homogenous. According to this model, softening behavior in the material results from the growth of voids, i.e. the model does not possess the intrinsic ability to predict localized deformation by void coalescence.

The objective of this work is to investigate the influence of damage mechanisms on localized deformation of amorphous glassy polymers. Here, damage is ascribed to the distributed growth of void volume and crazing during plastic deformation. The concept of free volume is employed to describe the voids or the loosely packed regions in amorphous glassy polymers. In contrast to rubber-toughened polymers, the void is considered as conceptual with no clear physical interpretation. However, since the voids are uniformly distributed in the material, the growth of voids is approximated by using the models which are conventionally applied to the modeling of void growth due to cavitation of small rubber particles or impurities present in polymer–rubber blends, cf. e.g. [19].

The specific model employed in this work is based on the celebrated 8-chain version of the [27] model, which is here termed the BPA model. In this Extended BPA (EBPA) model, both the elastic and plastic properties are considered as viscous. In order to evaluate the model predictions for inhomogeneous deformation, cold drawing experiments on PC were performed and the model was implemented in a finite element program. The EBPA model was calibrated to the