International Journal of Solids and Structures 51 (2014) 2765–2776

Contents lists available at ScienceDirect

International Journal of Solids and Structures

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

Formulation of a damage internal state variable model for amorphous glassy polymers

D.K. Francis [a,b,*], J.L. Bouvard [a,c], Y. Hammi [a], M.F. Horstemeyer [a,b]

[a] Center for Advanced Vehicular Systems, Mississippi State University, MS 39762, United States
[b] Department of Mechanical Engineering, Mississippi State University, PO Box ME, MS 39762, United States
[c] Mines–ParisTech, CEMEF, UMR 7635, BP 207, 06904 Sophia Antipolis cedex, France

ARTICLE INFO

Article history:
Received 8 February 2013
Received in revised form 14 March 2014
Available online 8 April 2014

Keywords:
Damage modeling
Thermoplastics
Constitutive behavior
Internal state variable

ABSTRACT

The following article proposes a damage model that is implemented into a glassy, amorphous thermoplastic thermomechanical inelastic internal state variable framework. Internal state variable evolution equations are defined through thermodynamics, kinematics, and kinetics for isotropic damage arising from two different inclusion types: pores and particles. The damage arising from the particles and crazing is accounted for by three processes of damage: nucleation, growth, and coalescence. Nucleation is defined as the number density of voids/crazes with an associated internal state variable rate equation and is a function of stress state, molecular weight, fracture toughness, particle size, particle volume fraction, temperature, and strain rate. The damage growth is based upon a single void growing as an internal state variable rate equation that is a function of stress state, rate sensitivity, and strain rate. The coalescence internal state variable rate equation is an interactive term between voids and crazes and is a function of the nearest neighbor distance of voids/crazes and size of voids/crazes, temperature, and strain rate. The damage arising from the pre-existing voids employs the Cocks–Ashby void growth rule. The total damage progression is a summation of the damage volume fraction arising from particles and pores and subsequent crazing. The modeling results compare well to experimental findings garnered from the literature. Finally, this formulation can be readily implemented into a finite element analysis.

1. Introduction

Continuum damage modeling used in finite element analysis of polymers is a quickly expanding area of interest as polymers are being viewed as a competitor to some metals for lightweighting designs. As such, the demand for more accurate material models is warranted (see Bouvard et al., 2009). For a review of the multiscale aspects of amorphous polymers, please see Boyce and Arruda (2000) for rubber constitutive modeling or Horstemeyer and Bammann (2010) for internal state variable theory for inelasticity). Part of the demand for more accurate modeling requires including appropriate damage progression effects.

However, the bulk of modeling damage in polymers employs the classic work by Gurson (1977). Lazzeri and Bucknall (1993, 1995) proposed and applied a modified Gurson model to rubber-toughened polymers to account for dilatational yielding. Jeong and Pan (1995) generalized Gurson's yield criterion to take into account pressure sensitivity, which reduced to Coulomb's yield criterion when the void volume fraction was zero. Later, Jeong (2002) implemented the same model into a finite element (FE) code and also added tensile hydrostatic pressure effects. To account for rupture due to vapor pressure in polymer electronic packages components, Guo and Cheng (2002) implemented the modified Gurson–Tvergaard model (Tvergaard, 1989), which calls a microscopic stress tensor and the void volume fraction as internal variables, into an FE code. Damage in rubber-modified epoxies was modeled by both Kody and Lesser (1999) and Imanaka et al. (2003) with Gurson constitutive equations. Because the Gurson formulation was originally applied to metals which fracture at small strains compared to ductile polymers, the yield stress is overestimated. Therefore, Pijnenburg and der Giessen (2001) modified it to account elasticity effects and shear banding. This same issue of large strains is also dealt with in Steenbrink et al. (1997) and Steenbrink and van der Giessen (1997). Recently, Zaïri et al. (2008) extended the Bodner–Partom model (Bodner and Partom, 1975) with a modified Gurson model (Tvergaard, 1981) in a thorough experimental/computational approach. Challier et al. (2006)

* Corresponding author at: Predictive Design Technologies, 60 Technology Blvd, STE 115B, Starkville, MS 39759, United States. Tel.: +1 6629950738.
E-mail address: dfrancis@predictivedesigntech.com (D.K. Francis).

http://dx.doi.org/10.1016/j.ijsolstr.2014.03.025
0020-7683/

studied polyvinylidene fluoride (PVDF) fracture mechanisms and then used the mechanical testing and microscopic observations to fit the Gurson–Tvergaard–Needleman (GTN) model (Tvergaard, 1982; Tvergaard and Needleman, 1984) in an FE analysis. Laiarinandrasana et al. (2009) studied PVDF as well but at lower temperatures, which drastically altered the mechanical response, yet they fit the GTN model to correspond to the material properties' temperature dependence following Khan et al. (2006). The GTN model was also compared to Bridgman tests to capture triaxiality effects in polyamide by Boisot et al. (2011).

Other failure criteria, apart from Gurson, have been developed as well for polymers. Gearing and Anand (2004a) employed two parameters into an FE analysis to distinguish between brittle and ductile failure, where once a critical strain was reached in an element, it was removed. To model crazing and molecular chain-scission related failure, a similar failure criterion was used by Gearing and Anand (2004b) where craze breakdown or molecular chain-scission occurred when a critical strain value was reached.

The following work proposes a damage framework that includes three mechanisms: damage from pores, damage from particles, and crazing. Crazing in this context is the organized fibrillar microstructure with lines of voids perpendicular to the principle tensile stress resulting from weak imperfections in the molecular composition. The damage from particles and crazes will be defined by separate void nucleation, growth, and coalescence rate equations that are included in a modified inelastic amorphous glassy thermoplastic internal state variable (ISV) model (Bouvard et al., 2013). The organizational structure of this study is as follows: First, the kinematics will be prescribed beginning with a multiplicative decomposition of the deformation gradient. Next, the thermodynamic restrictions as given by Coleman and Gurtin (1967) are followed to where a temperature evolution is found. Finally, the kinetics and constitutive model is proposed. Within the section, the damage evolution equations are given, and a void nucleation evolution model is developed. The notion is that this ISV model would be able to be employed within a finite element code.

1.1. Notation

Standard notation will be followed in this formulation. Tensors are denoted by boldface font while scalar values will have the standard weight. For example, the scalar product, C, of tensors A and B appears as $\boldsymbol{A}:\boldsymbol{B}=C$. Special care is given to specify configurations throughout the derivation by using accent marks where the tilde ($\tilde{\mathcal{B}}$), circumflex ($\hat{\mathcal{B}}$), and macron ($\bar{\mathcal{B}}$) represent different intermediate configurations. The following definitions are used in the text: $\boldsymbol{AB}\Rightarrow(\boldsymbol{A}\cdot\boldsymbol{B})_{ij}=A_{ik}B_{kj}$, $\boldsymbol{a}\otimes\boldsymbol{b}\Rightarrow(\boldsymbol{a}\otimes\boldsymbol{b})_{ij}=a_ib_j$, $\boldsymbol{A}:\boldsymbol{B}=A_{ij}B_{ij}$, and $\|\boldsymbol{A}\|=(A_{ij}A_{ij})^{1/2}$.

2. Kinematics

For a continuous three dimensional body in its initial state, any arbitrary point $\boldsymbol{X}$ can be mapped smoothly to a corresponding point, $\boldsymbol{x}$, in the current configuration using the deformation gradient tensor $\boldsymbol{F}$ along with a mapping function, $\boldsymbol{x}=\boldsymbol{\chi}(\boldsymbol{X},t)$, where

$$\boldsymbol{F}(\boldsymbol{X},t)=\frac{\partial\boldsymbol{\chi}(\boldsymbol{X},t)}{\partial\boldsymbol{X}} \tag{1}$$

Both points $\boldsymbol{X}$ and $\boldsymbol{x}$ are located in the same coordinate system (X_1,X_2,X_3), where $\boldsymbol{X}$ is the location of the point when time = 0 and $\boldsymbol{x}$ in the location of the point when time = t. The extended multiplicative decomposition of the deformation gradient tensor (Bilby et al., 1955; Kröner, 1958; Bammann et al., 1996) will take the following form:

$$\boldsymbol{F}=\boldsymbol{F}_{\mathrm{e}}\boldsymbol{F}_{\mathrm{t}}\boldsymbol{F}_{\mathrm{d}}\boldsymbol{F}_{\mathrm{p}} \tag{2}$$

In Eq. (2), each individual deformation gradient represents a physical deformation phenomenon. The elastic deformation gradient tensor, $\boldsymbol{F}_{\mathrm{e}}$, represents chain rotations and bond stretching that are reversible. The isotropic thermal deformation gradient tensor, $\boldsymbol{F}_{\mathrm{t}}$, represents deformation due to thermal expansion. The damage deformation gradient tensor, $\boldsymbol{F}_{\mathrm{d}}$, or volumetric inelastic deformation gradient, represents volumetric deformation due to increasing void volume. The plastic deformation gradient tensor, $\boldsymbol{F}_{\mathrm{p}}$, represents isochoric irreversible deformation.

There is no consensus on the placement of the thermal deformation gradient tensor, $\boldsymbol{F}_{\mathrm{t}}$; however, it is usually found either following the elastic deformation gradient (Weber and Boyce, 1989; Boyce et al., 1992; Arruda et al., 1995) or following the plastic deformation gradient (Bammann and Solanki, 2010; Bouvard et al., 2010). A physical basis for the latter can be made by considering a uniaxial tension test at room temperature interrupted prior to failure. The internal temperatures of thermoplastics generally rise during deformation. After unloading, the specimen is allowed to return to room temperature. The elastic deformation and the isotropic thermal expansion, is assumed to be negligible and the volumetric and deviatoric plastic deformation remains. Decomposing the total deformation gradient tensor into four separate deformation gradient tensors creates three intermediate configurations between the reference configuration, $\mathcal{B}_0$, and the current configuration, $\mathcal{B}$. The first intermediate configuration, $\tilde{\mathcal{B}}$, is defined by $\boldsymbol{F}_{\mathrm{p}}$. The second intermediate configuration, $\hat{\mathcal{B}}$, is defined by $\boldsymbol{F}_{\mathrm{d}}\boldsymbol{F}_{\mathrm{p}}$. The third intermediate configuration, $\bar{\mathcal{B}}$, is defined by $\boldsymbol{F}_\star$ where

$$\boldsymbol{F}_\star=\boldsymbol{F}_{\mathrm{t}}\boldsymbol{F}_{\mathrm{d}}\boldsymbol{F}_{\mathrm{p}},\quad \boldsymbol{F}=\boldsymbol{F}_{\mathrm{e}}\boldsymbol{F}_\star \tag{3}$$

The model is primarily expressed in the intermediate configuration of $\bar{\mathcal{B}}$ following Weber and Boyce (1989). The order of the deformation gradient tensors and configurations are visualized in Fig. 1.

The Jacobian of the deformation gradient tensor is the ratio of volume change for the previous configuration to the following configuration. For the damage deformation gradient, the Jacobian takes the following form:

$$J_{\mathrm{d}}=\det\boldsymbol{F}_{\mathrm{d}}=\frac{\widehat{V}}{\widetilde{V}} \tag{4}$$

Because of void nucleation, growth, and coalescence, the relationship between the volumes at $\tilde{\mathcal{B}}$ and $\hat{\mathcal{B}}$ are given by

$$\widehat{V}=V_{\mathrm{V}}+\widetilde{V} \tag{5}$$

where V_{V} is the volume of voids. Damage, ϕ, is defined as the ratio of the void volume to the total volume in $\hat{\mathcal{B}}$.

$$\phi=\frac{V_{\mathrm{V}}}{\widehat{V}} \tag{6}$$

Given Eqs. (4)–(6), assuming isotropic damage, the damage deformation gradient can thus be written in terms of ϕ as

$$J_{\mathrm{d}}=\frac{1}{1-\phi},\quad \boldsymbol{F}_{\mathrm{d}}=\frac{1}{(1-\phi)^{1/3}}\boldsymbol{1} \tag{7}$$

where $\boldsymbol{1}$ is a second rank identity tensor. The total Jacobian, which accounts for total volumetric change becomes

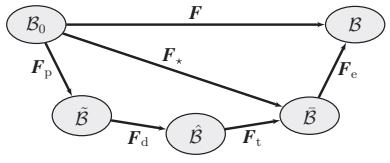

Fig. 1. Decomposition of the deformation gradient $\boldsymbol{F}$ into four components: deviatoric plastic $\boldsymbol{F}_{\mathrm{p}}$, volumetric plastic (damage) $\boldsymbol{F}_{\mathrm{d}}$, thermal $\boldsymbol{F}_{\mathrm{t}}$, and elastic $\boldsymbol{F}_{\mathrm{e}}$. $\boldsymbol{F}_\star$ represents the plastic-damage-thermal deformation gradient.