

A NUMERICAL ANALYSIS OF THE CRACK-TIP PLASTIC ZONE IN GLASSY POLYMERS

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This paper reports on a finite element analysis of the crack-tip plastic zone in viscoplastic glassy amorphous polymers. The constitutive model employed in this study accounts for the typical shear yielding behaviour of glassy polymers, i.e., the intrinsic softening upon yielding and the subsequent orientational strain hardening. The modified boundary layer approach is adopted to model the local finite-strain deformation processes around the crack. Numerical results show that the shape of the mode I plastic zone in glassy polymers depends greatly on the softening property of the material, and is quite different from that described by the Von Mises criterion for yielding in metals.

INTRODUCTION

There is an important class of polymers that can undergo substantial plastic deformation prior to fracture. Near the tip of a crack in such materials, the subsequent shielding by the plastic zone can strongly influence the fracture resistance. Therefore, a proper description of the plastic deformation zone near the crack tip is vitally important for the understanding of the fracture mechanisms in these polymers. Much effort has been made to characterize the crack-tip plastic zone in metals. Contrary to this, the interpretation of the crack-tip deformation process in polymers is still at a speculative level with regard to a detailed understanding. This is mainly caused by the fact that polymers exhibit quite a different, and in many respects more complicated, plastic behaviour than metals.

It has been well recognized that glassy amorphous polymers exhibit plastic deformation below the glass transition temperature through the activation of microscopic shear bands, giving rise to a macroscopically viscoplastic response. Thus, the

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deformation behaviour is essentially rate-sensitive and temperature dependent. On the macroscopic scale, the localized inelastic deformation in polymers is rather different from that in metals owing to the intrinsic softening after yield followed by the increasing hardening. This particular constitutive behaviour is likely to be an important factor influencing the fracture of glassy polymers.

In the present paper, finite element computations are used for a basic investigation into the plastic zone near the crack tip in amorphous polymers under plane strain conditions. Computations are performed for two sets of material parameters which are representative for PC and PMMA, respectively.

MATERIAL MODEL

The material model employed in this study is based on the 3-D elastic-viscoplastic model for amorphous polymers proposed originally by Boyce et al. (1) and modified by Wu and Van der Giessen (2). This model incorporates the initial linear elastic response, the rate-dependent (visco-) plastic flow of the material, including intrinsic softening upon yielding, and nonlinear strain hardening at large plastic deformations. A brief recapitulation of the constitutive model is given here.

The strain rate \mathbf{D} is decomposed into an elastic part \mathbf{D}^e and a plastic part \mathbf{D}^p , i.e.

$$\mathbf{D} = \mathbf{D}^e + \mathbf{D}^p. \quad (1)$$

Assuming that the elastic strains remain small, the elastic strain rate \mathbf{D}^e can be described by the hypoelastic law

$$\mathbf{D}^e = \underline{\mathcal{L}}_e^{-1} \nabla \boldsymbol{\sigma}, \quad (2)$$

in terms of the Jaumann derivative of the Cauchy stress tensor $\boldsymbol{\sigma}$, $\nabla \boldsymbol{\sigma} = \dot{\boldsymbol{\sigma}} - \mathbf{W}\boldsymbol{\sigma} + \boldsymbol{\sigma}\mathbf{W}$, in which \mathbf{W} is the continuum spin tensor. Here, $\underline{\mathcal{L}}_e$ is the fourth-order isotropic elastic modulus tensor in terms of Young's modulus E and Poisson's ratio ν .

According to the Argon (3) model for plastic flow in glassy polymers, the equivalent plastic shear strain rate $\dot{\gamma}^p$ due to an applied shear stress τ is given by

$$\dot{\gamma}^p = \dot{\gamma}_0 \exp \left[-\frac{A s_0}{T} \left(1 - \left(\frac{\tau}{s_0} \right)^{5/6} \right) \right], \quad (3)$$

where $\dot{\gamma}_0$ and A are material parameters, T is the absolute temperature, and s_0 is the material shear strength. In order to incorporate the effect of pressure p on the plastic flow, and the effect of strain softening, s_0 in Eq. (3) is replaced with $s + \alpha p$. Here, s is assumed to evolve with plastic straining via $\dot{s} = h (1 - s/s_{ss}) \dot{\gamma}^p$, in which h is a material parameter and s_{ss} is the saturation value of s .

The plastic strain rate \mathbf{D}^p is thus expressed as

$$\mathbf{D}^p = \frac{\dot{\gamma}^p}{\sqrt{2}\tau} \bar{\boldsymbol{\sigma}}', \quad (4)$$

where τ is the equivalent shear stress, $\tau = \sqrt{(1/2) \bar{\boldsymbol{\sigma}}' \cdot \bar{\boldsymbol{\sigma}}'}$, and the driving stress $\bar{\boldsymbol{\sigma}}'$ is defined by

$$\bar{\boldsymbol{\sigma}}' = \boldsymbol{\sigma} - \mathbf{b}, \quad (5)$$

where \mathbf{b} is the back stress tensor accounting for the strain hardening of the material. On the basis of the description of the fully 3-D orientation distribution of molecular chains in a non-Gaussian network, Wu and Van der Giessen (2) derived the back stress \mathbf{b} in terms of its principal components b_α on the unit principal direction \mathbf{e}_α^p , corresponding to the principal plastic stretches λ_α , as follows,*

$$\mathbf{b} = \sum_{\alpha} b_{\alpha} (\mathbf{e}_{\alpha}^p \otimes \mathbf{e}_{\alpha}^p); \quad b_{\alpha} = b_{\alpha}(\lambda_{\beta}). \quad (6)$$

They further showed that their numerical computations can be captured very accurately by the following combination of the classical three-chain network description and the Arruda and Boyce eight-chain model (1):

$$b_{\alpha} = (1 - \rho) b_{\alpha}^{3\text{-ch}} + \rho b_{\alpha}^{8\text{-ch}}, \quad (7)$$

with ρ being determined by the maximum plastic stretch $\bar{\lambda} = \max(\lambda_1, \lambda_2, \lambda_3)$ through $\rho = 0.85\bar{\lambda}/\sqrt{N}$. Here, N is a statistical parameter determining the limit stretch λ_{\max} of a molecular chain as $\lambda_{\max} = \sqrt{N}$. The principal back stress components are given by

$$b_{\alpha}^{3\text{-ch}} = \frac{1}{3} C^R \sqrt{N} \lambda_{\alpha} \mathcal{L}^{-1} \left(\frac{\lambda_{\alpha}}{\sqrt{N}} \right) \quad (8)$$

$$b_{\alpha}^{8\text{-ch}} = \frac{1}{3} C^R \sqrt{N} \frac{\lambda_{\alpha}^2}{\lambda_c} \mathcal{L}^{-1} \left(\frac{\lambda_{\alpha}}{\sqrt{N}} \right); \quad \lambda_c^2 = \frac{1}{3} \sum_{\beta=1}^3 \lambda_{\beta}^2, \quad (9)$$

where C^R is a material constant and \mathcal{L} denotes the Langevin function defined as $\mathcal{L}(\beta) = \coth\beta - 1/\beta$. When the value of either $\bar{\lambda}$ or λ_c exceeds $0.99\lambda_{\max}$, the network is 'locked' and no further viscoplastic flow is allowed.

PROBLEM FORMULATION AND NUMERICAL IMPLEMENTATION

Confining to the framework of small-scale yielding, the modified boundary layer approach is employed to study the mode I plastic zone near an initially blunted crack tip with a radius of 0.1 mm, under plane strain conditions. Finite strains are accounted for, and the governing equations are formulated using convected coordinates. The remote displacement components u_1 and u_2 , with respect to the undeformed

* Throughout this paper, the summation convention is *not* implied for Greek indices.

base vector, are specified in terms of the stress intensity factor K_1 through the elastic field

$$u_1 = 2(1 + \nu) \frac{K_1}{E} \sqrt{\frac{r}{2\pi}} \cos \frac{\theta}{2} \left[2 - 2\nu - \left(\cos \frac{\theta}{2} \right)^2 \right], \quad (10)$$

$$u_2 = 2(1 + \nu) \frac{K_1}{E} \sqrt{\frac{r}{2\pi}} \sin \frac{\theta}{2} \left[2 - 2\nu - \left(\cos \frac{\theta}{2} \right)^2 \right], \quad (11)$$

where r and θ are polar coordinates with the origin located at the crack tip.

The problem is analysed numerically by means of a finite element discretization of the governing finite strain field equations using a Total Lagrangian formulation. Quadrilateral elements are used, each of which is built up of four linear velocity, triangular subelements arranged in a 'crossed triangle' configuration. The solution of the problem is obtained on the basis of a linear incremental form of the virtual work principle. In each computation the loading (K_1) is increased linearly at a rate of $35 \text{ Nmm}^{-3/2} \text{ s}^{-1}$, corresponding to an isothermal deformation process in a tensile test of practical specimens at a loading speed of the order of $\sim 10^{-4} \text{ m/s}$. During the incremental procedure an equilibrium correction procedure is employed to avoid drifting away from the true equilibrium path. Furthermore, we use an adaptive time stepping method proposed by Wu and Van der Giessen (4).

RESULTS

Here a few results are shown for two sets of material parameters, that exhibit typical features for PC and PMMA, respectively, at room temperature ($T = 294 \text{ K}$). Table 1 lists all parameters. The stress-strain behaviour of PC and PMMA under uniaxial tension is displayed in Figure 1. A distinct difference between the constitutive behavior of these two materials is that PMMA exhibits much less intrinsic strain softening after yielding than PC.

Figures 2 and 3 show the active crack-tip plastic zones in PC and PMMA, respectively, at an instant when the applied load K_1 is $130 \text{ Nmm}^{-3/2}$. This is indicated by contours of the instantaneous plastic shear rate $\dot{\gamma}^p$. It is seen that the contour of the plastic zone in PMMA has some resemblance to that in metals. Near the crack tip in PC, however, the shape of the plastic zone is flattened, which is completely different from that predicted by the Von Mises criterion in metals. In fact, the shape of the plastic zone is controlled primarily by the occurrence of the shear band (Figure 2), which has propagated through the tip region during loading. In view of the magnitude of the plastic shear rate $\dot{\gamma}^p$ as well as the shape of the plastic zone, the plastic deformation in PC is seen to be more intensive and more localised than that in PMMA. This deviation of the plastic deformation processes near the crack tip in polymers compared to that in metals, which exhibit no strain softening upon yielding, is caused by the intrinsic softening behaviour of polymers.

Table 1. Material parameters

	ν	E/s_0	s_{ss}/s_0	As_0/T	h/s_0	N	C^R
PC	0.4	9.38	0.79	79.2	5.15	2.8	0.132
PMMA	0.4	9.38	0.92	79.2	5.15	2.8	0.132

The results obtained in this work will be instrumental for future attempts to describe the crack initiation and propagation in polymers and polymer blends.

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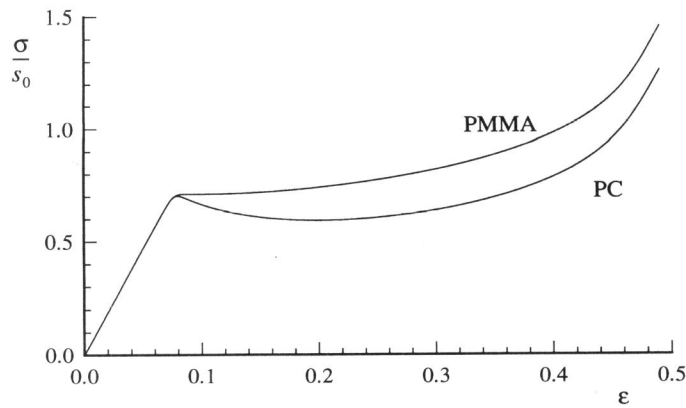


Figure 1 True stress vs. logarithmic strain curve in uniaxial tension for PC and PMMA type materials at $\dot{\epsilon} = 0.001$.

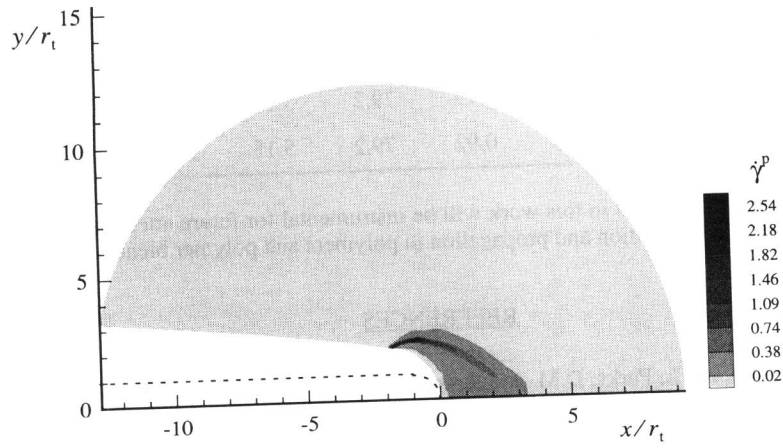


Figure 2 The active crack-tip plastic zone in PC at $K_I = 130\text{Nmm}^{-3/2}$. The coordinates are normalised by the initial crack-tip radius r_t . The dashed line indicates the initial blunted crack.

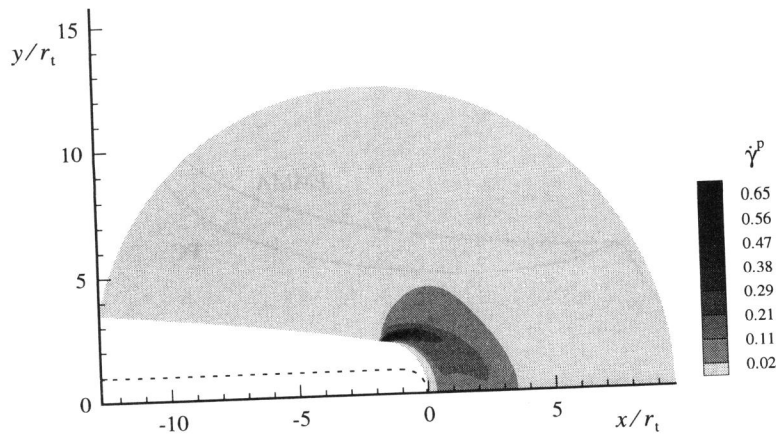


Figure 3 The active crack-tip plastic zone in PMMA at $K_I = 130\text{Nmm}^{-3/2}$. The coordinates are normalised by the initial crack-tip radius r_t . The dashed line indicates the initial blunted crack.