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ON NECK PROPAGATION IN AMORPHOUS GLASSY POLYMERS UNDER PLANE STRAIN TENSION

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Abstract—Unlike metals, necking in polymers under tension does not lead to further localization of deformation, but to propagation of the neck along the specimen. Finite element analysis is used to numerically study necking and neck propagation in amorphous glassy polymers under plane strain tension during large strain plastic flow. The constitutive model used in the analyses features strain-rate, pressure, and temperature dependent yield, softening immediately after yield and subsequent orientational hardening with further plastic deformation. The latter is associated with distortion of the underlying molecular network structure of the material, and is modelled here by adopting a recently proposed network theory developed for rubber elasticity. Previous studies of necking instabilities have almost invariably employed idealized prismatic specimens; here, we explicitly account for the unavoidable grip sections of test specimens. The effects of initial imperfections, strain softening, orientation hardening, strain-rate as well as of specimen geometry and boundary conditions are discussed. The physical mechanisms for necking and neck propagation, in terms of our constitutive model, are discussed on the basis of a detailed parameter study.

I. INTRODUCTION

Necking and neck propagation are typical examples of plastic instability phenomena in amorphous glassy polymers. Although our understanding of plastic instabilities appears to come primarily from research on polycrystalline metals and soils, a number of characteristic aspects of localization instabilities in polymers begins to be assessed (see e.g. BOWDEN [1973], G'SELL [1986], BOYCE *et al.* [1992], WU & VAN DER GIESSEN [1994]). It is now widely acknowledged that glassy polymers exhibit plastic deformation below the glass transition temperature mainly through the activation of microscopic shear bands. On the macroscopic scale, it is well known that macroscopic strain localization in polymers can be very different from that in metals due to the dramatic stiffening of polymers at large strains. Although plastic instabilities like necks or shear bands in metals almost invariably tend to localize progressively until failure intervenes, necks and macroscopic shear bands in polymers typically do not continue to localize but tend to propagate along the specimen (see e.g. G'SELL & JONAS [1979], G'SELL & GOPEZ [1985], NEALE & TUGCU [1985, 1987a, b], BOYCE & ARRUDA [1990], WU & VAN DER GIESSEN [1994]).

Neck propagation, or commonly termed cold drawing, is a standard technique used to orient the molecular chains of the polymers and thereby to harden the polymer of products such as fibres (axisymmetric deformation) and magnetic tape and sheet materials (plane strain deformations). Cold drawing has been studied experimentally for instance by G'SELL and co-workers (see e.g. G'SELL & JONAS [1979], MARQUEZ-LUCERO *et al.* [1989], and G'SELL *et al.* [1992]). Except under conditions of very slow neck propagation, frictional heating of the polymer undergoing large deformations brings ther-

mododynamic considerations into the problem (see e.g. BOYCE *et al.* [1992]). However, the phenomenon of neck propagation is in essence a mechanical one, and therefore the problem is usually considered as a quasi-static deformation problem under isothermal conditions.

COLEMAN [1983] and HUTCHINSON and NEALE [1983] consider the ideal steady-state phase of neck propagation. For a nonlinear elastic solid described by J_2 deformation theory, HUTCHINSON and NEALE [1983] determined the states on both sides of the neck from the jump conditions (across the neck) that result from conservation of mass, momentum, and energy. An approximate solution was given for an elastic-plastic solid described by J_2 flow theory that was based on introducing a parameterized stream function into a variational principle. Subsequently, full finite element analyses have been carried out for axisymmetric neck propagation (NEALE & TUGCU [1985], TOMITA *et al.* [1990]) and for plane strain neck propagation (FAGER & BASSANI [1986], TUGCU & NEALE [1987a]). The effects of strain rate sensitivity (TUGCU & NEALE [1987a, 1987b, 1988]), and kinematic hardening (TUGCU & NEALE [1987a]) on neck propagation behaviour have also been investigated.

The constitutive models used in the above-mentioned studies are rather simple and entirely phenomenological. In most studies, the hardening response was simply chosen to fit the characteristic uniaxial stress-strain response of highly deformable, (semi-)crystalline polymers. Potentially more accurate constitutive models, based on detailed micro-mechanical considerations, have appeared very recently. In this article we focus on the class of amorphous glassy polymers for which, on the one hand, the more phenomenological constitutive models used in previous necking studies do not apply, and for which on the other hand more physically based models have appeared recently. Using the 3-D constitutive model for amorphous glassy polymers proposed by BOYCE *et al.* [1988], BOYCE and ARRUDA [1990] studied the large strain tensile response of glassy polymers. Although the predicted true stress-strain curve was found to accurately capture the observed test data, the kinetics of necking and neck propagation was not discussed in their article.

The fully 3-D constitutive model for amorphous glassy polymers, proposed originally by BOYCE *et al.* [1988] and modified by WU and VAN DER GIESSEN [1993a], has been found to be able to predict many aspects of the large plastic strain behaviour of glassy polymers observed experimentally (WU & VAN DER GIESSEN [1993a, 1993b, 1994]). In a recent study, a finite element simulation of shear band propagation in glassy polymers during plane strain simple shear was carried out (WU & VAN DER GIESSEN [1994]), focusing attention on the initiation and propagation of the shear band. The numerical results showed that the shear band propagation phenomenon could be captured by the type of constitutive models available now. In this article, the constitutive model is incorporated in finite element simulations of the plane strain tension of amorphous glassy polymers, focusing attention on the initiation of necking and neck propagation along the specimen. Results are given for the overall load-elongation response and the thickness reduction-elongation response of the specimen. In some cases the deformed meshes and the distributions of plastic strain rate at various deformation stages are provided. Based on the detailed parameter analyses, the mechanisms of necking and neck propagation are discussed in some detail.

Tensors will be denoted by bold-face letters. The tensor product is denoted by $\otimes$, and the following operations for second and fourth-order tensors apply ($\mathbf{a} = a_{ij}\mathbf{e}_i \otimes \mathbf{e}_j$, $\mathbf{b} = b_{ij}\mathbf{e}_i \otimes \mathbf{e}_j$, $\mathbf{A} = A_{ijkl}\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l$, $\mathbf{e}_i$ being a Cartesian basis): $\mathbf{ab} = a_{ik}b_{kj}\mathbf{e}_i \otimes \mathbf{e}_j$ and $\mathbf{Ab} = A_{ijkl}b_{kl}\mathbf{e}_i \otimes \mathbf{e}_j$. Superscripts T and -1 denote the transverse and inverse of

a second-order tensor, respectively. The trace is denoted by tr , and a superposed dot denotes the material time derivative or rate. The deviatoric part of a second-order tensor $\mathbf{a}$ is denoted by a prime, that is, $\mathbf{a}' = \mathbf{a} - (\text{tr } \mathbf{a}/3)\mathbf{I}$, with $\mathbf{I}$ being the unit tensor.

II. CONSTITUTIVE EQUATIONS

In this section, we briefly recapitulate the constitutive framework we are going to adopt throughout this article, mainly for the purpose of definition and notation. For details we refer to BOYCE *et al.* [1988] and WU and VAN DER GIESSEN [1993a]. It is assumed that before large strain inelastic flow may occur a glassy polymer must overcome two physical distinct sources of resistance: (a) an intermolecular resistance to segment rotation; and (b) an anisotropic internal resistance due to molecular alignment.

ARGON [1973] has developed a relatively simple model for plastic flow made possible by the cooperative rotation of segments. According to this model, the plastic shear strain rate $\dot{\gamma}^p$ due to an applied shear stress τ is given by

$$\dot{\gamma}^p = \dot{\gamma}_0 \exp \left[-\frac{As_0}{T} \left(1 - \left(\frac{\tau}{s_0} \right)^{5/6} \right) \right]. \quad (1)$$

Here, $\dot{\gamma}_0$ is a preexponential factor, A is a material parameter that is proportional to the activation volume/Boltzmann's constant, T is the absolute temperature, and s_0 is the athermal shear strength, which in Argon's model is given by $s_0 = 0.077 \mu / (1 - \nu)$ in terms of the elastic shear modulus μ and Poisson's ratio ν . BOYCE *et al.* [1988] extended this expression to include the effect of the pressure p by using $s + \alpha p$ instead of s_0 , where α is a pressure dependence coefficient. Furthermore, they accounted for intrinsic softening by assuming s to evolve with plastic straining via

$$\dot{s} = h(1 - s/s_{ss})\dot{\gamma}^p, \quad (2)$$

where h is the rate of resistance drop with respect to the plastic strain and s_{ss} is the assumed saturation value of s .

During continued plastic flow, the molecular chains will tend to align along the direction of principal plastic stretch (see e.g. HAWARD & THACKRAY [1968]). This molecular "texture" development tends to decrease the configurational entropy of the system, which, in turn, creates an internal network stress. This process of network distortion is very similar to that of rubber network, and HAWARD and THACKRAY [1968] suggested to describe this for uniaxial extension by means of a back stress determined through a Langevin spring, as suggested by non-Gaussian network theory. BOYCE *et al.* [1988] extended this approach to general three-dimensional plastic deformations by introducing a back stress tensor $\mathbf{B}$, which is taken to be coaxial with the plastic left stretch tensor $\mathbf{V}^p$ (the determination of $\mathbf{V}^p$ in the complete constitutive framework will be discussed later). Thus, if $\mathbf{e}_i^p$ are the unit eigenvectors of $\mathbf{V}^p$, corresponding to a plastic stretch λ_i^p , the back stress $\mathbf{B}$ is constructed as

$$\mathbf{B} = \sum_i B_i (\mathbf{e}_i^p \otimes \mathbf{e}_i^p) \quad (3)$$

from the principal components B_i . Originally, BOYCE *et al.* [1988] adopted the classical so-called three-chain model for which the principal components $B_i^{3\text{-ch}}$ of the back stress tensor are given in terms of the plastic stretches λ_i^p by (see WANG & GUTH [1952])

$$B_i^{3-ch} = \frac{1}{3} C^R \sqrt{N} \left[\lambda_i^p \mathcal{L}^{-1} \left(\frac{\lambda_i^p}{\sqrt{N}} \right) - \frac{1}{3} \sum_{j=1}^3 \lambda_j^p \mathcal{L}^{-1} \left(\frac{\lambda_j^p}{\sqrt{N}} \right) \right] \quad (\text{no sum over } i), \quad (4)$$

where C^R is known as the rubbery modulus, N is a statistical network parameter related to the network locking stretch, and $\mathcal{L}$ is the Langevin function defined by $\mathcal{L}(\beta) = \coth \beta - 1/\beta$.

Later, ARRUDA and BOYCE [1991,1993a,b] found that the three-chain non-Gaussian network model was not capable of picking up the strain hardening observed experimentally in polycarbonate (PC) and polymethylmetacrylate (PMMA). They suggested to model the network by the so-called eight-chain model, which considers a set of eight chains connecting the central junction point and each of the eight corners of the unit cube. The principal components of the back stress tensor according to this eight-chain non-Gaussian network model are given by

$$B_i^{8-ch} = \frac{1}{3} C^R \sqrt{N} \mathcal{L}^{-1} \left(\frac{\lambda^p}{\sqrt{N}} \right) \frac{\lambda_i^{p^2} - \lambda^{p^2}}{\lambda^p}, \quad \lambda^{p^2} = \frac{1}{3} \sum_{j=1}^3 \lambda_j^{p^2}. \quad (5)$$

More close agreement with the experimental results for PC and PMMA has been obtained by ARRUDA and BOYCE [1991,1993a,b] based on the eight-chain model.

Obviously, the eight-chain model is but an approximate representations of the actual spatial distributions of molecular chains by “lumping” their orientations in eight specific directions. Furthermore, the eight-chain model is expected to underestimate the stiffness of the network. Very recently, the authors developed the so-called full network model in which full account is taken of the 3-D orientation distribution of the individual chains in the network (WU & VAN DER GIESSEN [1992,1993a]). The principal back stresses according to this model can be given by

$$B_i = \frac{1}{4\pi} C^R \sqrt{N} \int_0^\pi \int_0^{2\pi} \mathcal{L}^{-1} \left(\frac{\lambda^p}{\sqrt{N}} \right) \frac{\lambda_i^{p^2} m_i^{0^2} - \lambda^{p^2}/3}{\lambda^p} \sin \theta_0 d\theta_0 d\varphi_0 \quad (\text{no sum over } i). \quad (6)$$

Here, λ^p is defined by

$$\lambda^{p^2} = \sum_{j=1}^3 \lambda_j^{p^2} m_j^{0^2},$$

and m_i^0 are the unit vector components in orientation space defined by

$$m_1^0 = \sin \theta_0 \cos \varphi_0, \quad m_2^0 = \sin \theta_0 \sin \varphi_0, \quad m_3^0 = \cos \theta_0$$

in terms of the angles θ_0 and φ_0 , which measure the orientation of molecular chains relative to the principal stretch directions in the undeformed configuration. The numerical evaluation of the integral in (6) is rather time-consuming, but an accurate approximation of the full network predictions according to (6) has been found (WU &

VAN DER GIESSEN [1992]) in the form of a combination of the three-chain and eight-chain model predictions (4), (5) through

$$B_i = (1 - \rho^p) B_i^{3-ch} + \rho^p B_i^{8-ch}. \quad (7)$$

Excellent agreement with full integration is obtained by taking ρ^p to be related to the maximum principal plastic stretch $\lambda_{\max}^p = \max(\lambda_1^p, \lambda_2^p, \lambda_3^p)$ via $\rho^p = 0.85 \lambda_{\max}^p / \sqrt{N}$. All computations to be reported here have used the expression (7).

The complete tensorial form of the constitutive model has been developed by BOYCE *et al.* [1988], in which the deformation gradient $\mathbf{F}$ is multiplicatively decomposed into elastic and plastic parts, $\mathbf{F} = \mathbf{F}^e \mathbf{F}^p$. With no loss of generality, the elastic part $\mathbf{F}^e$ is taken to be symmetric, so that $\mathbf{F}^p$ represents the relaxed configuration obtained by unloading without rotation (in the polar decomposition sense). According to this decomposition, the velocity gradient $\mathbf{L}$ is decomposed as

$$\mathbf{L} = \dot{\mathbf{F}} \mathbf{F}^{-1} = \mathbf{D} + \mathbf{W} = \dot{\mathbf{F}}^e \mathbf{F}^{e-1} + \mathbf{F}^e \mathbf{L}^p \mathbf{F}^{e-1},$$

where $\mathbf{D}$ is the rate of deformation, $\mathbf{W}$ is the spin, and $\mathbf{L}^p = \mathbf{D}^p + \mathbf{W}^p = \dot{\mathbf{F}}^p \mathbf{F}^{p-1}$ is the velocity gradient in the relaxed configuration. With the adopted symmetry of $\mathbf{F}^e$, the skewsymmetric part $\mathbf{W}^p$ is algebraically given as $\mathbf{W}$ plus a term dependent on $\mathbf{F}^e$ and $\mathbf{D} + \mathbf{D}^p$ (BOYCE *et al.* [1988]). Because the elastic strains will remain small, we can neglect geometry differences between current and relaxed configurations. Thus, the constitutive equations can be simplified significantly. In particular it is noted that in this case $\mathbf{W}^p \approx \mathbf{W}$ and $\mathbf{D} \approx \mathbf{D}^e + \mathbf{D}^p$, with $\mathbf{D}^e$ the symmetric part of $\dot{\mathbf{F}}^e \mathbf{F}^{e-1}$ (see BOYCE *et al.* [1988]).

The magnitude of the strain rate $\mathbf{D}^p$ (the rate of shape change of the relaxed configuration) is taken to be given by the plastic shear strain rate, $\dot{\gamma}^p$, according to (1), while the tensor direction of $\mathbf{D}^p$ is specified by $\mathbf{N}$, so that

$$\mathbf{D}^p = \dot{\gamma}^p \mathbf{N}, \quad (8)$$

where the direction $\mathbf{N}$ is the deviatoric part of the driving stress, normalized by the effective equivalent shear stress τ :

$$\mathbf{N} = \frac{1}{\sqrt{2}\tau} \tilde{\boldsymbol{\sigma}}', \quad \tau = \sqrt{\frac{1}{2} \tilde{\boldsymbol{\sigma}}' \cdot \tilde{\boldsymbol{\sigma}}'}. \quad (9)$$

The driving stress $\tilde{\boldsymbol{\sigma}}$ itself is defined by

$$\tilde{\boldsymbol{\sigma}} = \boldsymbol{\sigma} - \mathbf{B}, \quad (10)$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor and $\mathbf{B}$ is the back stress tensor, according to (3) and (6) or (7). By observing that $\mathbf{V}^2 = \mathbf{F}^e (\mathbf{V}^p)^2 (\mathbf{F}^e)^T$ it is seen that, consistent with neglecting the elastic geometry changes ($\mathbf{F}^e \approx \mathbf{I}$), the plastic principal stretches λ_i^p to be substituted into (4–6) are approximated by the principal values of $\mathbf{V} \approx \mathbf{V}^p$.

The Cauchy stress is taken to be given by the elastic constitutive law with the hypo-

elastic rate form and employing the Jaumann stress rate, $\dot{\bar{\sigma}} = \dot{\sigma} - \mathbf{W}\sigma + \sigma\mathbf{W}$ to retain objectivity,

$$\dot{\bar{\sigma}} = \mathfrak{L}_e \mathbf{D}^e, \quad (11)$$

where $\mathfrak{L}_e$ is the fourth-order isotropic elastic modulus tensor:

$$\mathfrak{L}_e = \mathfrak{L}_e^{ijkl} \mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l, \\ \mathfrak{L}_e^{ijkl} = \frac{E}{2(1+\nu)} \left[(\delta^{ik}\delta^{jl} + \delta^{il}\delta^{jk}) + \frac{2\nu}{1-2\nu} \delta^{ij}\delta^{kl} \right], \quad (12)$$

with $E = 2(1+\nu)\mu$ being Young's modulus. The constitutive equations (11) can be finally arranged in the following form:

$$\dot{\bar{\sigma}} = \mathfrak{L}_e \mathbf{D} - \dot{\sigma}_v, \quad (13)$$

where $\dot{\sigma}_v = \mathfrak{L}_e \mathbf{D}^p$ acts as an instantaneous stress rate term that represents the viscoplastic contribution.

III. PROBLEM FORMULATION AND METHOD OF SOLUTION

We consider a tensile test specimen with grips as shown in Fig. 1, which has a gauge section with a rectangular cross-section. Contrary to most necking studies found in the literature, we do not just consider the prismatic gauge section, but also include the thicker grip sections. The reason for doing so is that after substantial neck propagation, the neck will approach the end of the gauge section and may then interact with the grips used to load the specimen. At that stage, velocity or strain fields at the interface between gauge section and grips become distorted, and it would be very difficult to accurately determine the boundary conditions for the gauge section.

In the initial configuration, the gauge section has a length $2B_0$ and a thickness $2A_0$. A Cartesian coordinate system with $x_1 = x$, $x_2 = y$, $x_3 = z$ is used as a reference, in which x is associated with the loading direction, while y refers to the thickness direc-

Fig. 1. Schematic definition of the plane strain tension specimen (only one quadrant is shown).

tion. The transition from the gauge section thickness $2A_0$ to the grip thickness $2H_0$ occurs over a length L_e , and is for simplicity described analytically by

$$y = A_0 + (H_0 - A_0) \left(1 - \frac{\arctan \left(Q \frac{L_e + B_0 - x}{L_e} \right)}{\arctan Q} \right), \quad B_0 \leq x \leq (B_0 + L_e),$$

where the parameter Q determines how steep the transition is. The elongation in the gauge section is commonly expressed by the ratio $\epsilon = U_g/B_0$, where the gauge section displacement U_g is determined as the average displacement over the section $x = B_0$ in the initial configuration. The specimen is deformed by imposing the displacement rate $\dot{U}$ in the x direction at the free end without restraining the lateral movement so that the rate boundary conditions at $x = L_0$ become

$$T^y(L_0, y) = 0, \quad \dot{u}_x(L_0, y) = \dot{U}, \quad (14)$$

where T^y is the nominal traction vector component in y direction. Thus the loading is displacement controlled and the grip surface $x = L_0$ is shear free. From symmetry about $x = 0$, we have

$$T^y(0, y) = 0, \quad \dot{u}_x(0, y) = 0. \quad (15)$$

The strain rate in the gauge section is approximately defined by $\dot{\epsilon} = \dot{U}/B_0$. The lateral surfaces of the specimen are taken to be stress-free. Variations of the width (in z direction) during the deformation are neglected; thus, the deformation is plane strain. The conventional nominal stress or engineering stress is defined by $F_x/(2A_0)$, where F_x is the applied tensile force. Furthermore, we define a thickness-reduction ratio $\kappa = A_N/A_0$ at the minimum section, which for the present problem always coincides with $x = 0$. Because of the symmetry with respect to the mid-planes $x = 0$, $y = 0$, only one quadrant of the symmetry specimen needs to be analyzed (see Fig. 1).

In most experiments and perhaps all numerical simulations (see e.g. G'SELL & JONAS [1979], NEALE & TUGCU [1985, 1987a, b]), an initial "geometric" imperfection was used to trigger the initiation of the neck. However, in the experiments carried out by G'SELL *et al.* [1992] and G'SELL and MARQUEZ-LUCERO [1993], a predeformation defect was introduced centrally in each specimen by folding and defolding the specimen locally. It was shown that such a "mechanical" defect acts as an efficient neck initiator in those cases where a neck is likely to be formed (G'SELL & MARQUEZ-LUCERO [1993]). To trigger the initiation of the neck at the mid-plane $x = 0$ of the specimen in our numerical analysis, we assume here an initial mechanical imperfection of the shear strength s_0 of the form

$$\Delta s_0 = \zeta s_0 \cos \frac{\pi x}{L_0} \quad (16)$$

such that the actual initial shear strength is $s_0 - \Delta s_0$, where ζ determines the intensity of the imperfection.

A numerical analysis is performed by employing a finite element scheme in a manner similar to that described by NEEDLEMAN and TVERGAARD [1984]. We use quadrilateral elements, each built up of four linear velocity, triangular subelements arranged in

a "crossed triangle" configuration. The initiation and propagation of the shear bands has been observed during large strain deformations in amorphous glassy polymers (see e.g. WU & TURNER [1973], G'SELL & GOPEZ [1985]), where the element size defines the minimum possible thickness of the shear band (TVERGAARD *et al.* [1981]). Therefore, an analysis with a fine mesh could result in a narrower shear band. The shear band will form along element boundaries. The quadrilateral element mesh formation provides a greater freedom for the deformation to localize because of the large number and direction of element boundary (TVERGAARD *et al.* [1981]). An equilibrium correction procedure is employed in this analysis to avoid drifting away from the true equilibrium path during the incremental procedure. Integrations with respect to time are computed, for the time being, by using an explicit Euler integration method. Because, according to eqn (13), the elements of the stiffness mixture are of the order of the elastic moduli, very small time steps have to be employed to achieve satisfactory accuracy. This applies definitely in the early stages of viscoplastic flow, but at later stages of well-developed viscoplastic flow, much large steps may be used. For this reason we use an adaptive time stepping method proposed very recently by VAN DER GIESSEN and NEALE [1993] and used in the numerical simulations of shear band propagation at large plane strain simple shear by WU and VAN DER GIESSEN [1994], in which the time step size Δt to be used for each increment is determined adaptively. The procedure uses a number of criteria that ensure that the shear stress drop and the plastic shear strain increment during a time increment remain within user-defined bounds. The procedure is rather heuristic, but extremely simple to implement in an incremental code. By employing this simple adaptive time stepping scheme we have been quite efficient in obtaining stable solutions with acceptable numbers of increments. For further details concerning the finite element method, we refer to WU and VAN DER GIESSEN [1994].

IV. RESULTS

The problem described in Sec. III involves a number of dimensionless groups, and therefore we introduce the following nondimensional quantities:

$$\text{loading:} \quad \epsilon = \frac{U_g}{B_0}, \quad \sigma = \frac{F_x}{2A_0s_0}, \quad \kappa = \frac{A_N}{A_0}, \quad \frac{\dot{\epsilon}}{\sqrt{3}\dot{\gamma}_0}; \quad (17)$$

$$\text{geometry:} \quad B_0/A_0, \quad L_0/B_0, \quad L_e/L_0, \quad H_0/A_0, \quad Q; \quad (18)$$

$$\text{material:} \quad \frac{E}{s_0}, \quad \frac{s_{ss}}{s_0}, \quad \frac{As_0}{T}, \quad \frac{h}{s_0}, \quad \nu, \quad \alpha, \quad N, \quad \frac{C^R}{s_0}. \quad (19)$$

The overall response of the specimen can be conveniently presented in terms of the applied elongation ϵ , and the normalized nominal stress σ , and the thickness-reduction ratio κ at the minimum section ($x = 0$).

IV.1. A typical result

Fig. 2 shows the predicted response for specimen dimensions specified by $B_0/A_0 = 4$, $L_0/B_0 = 2$, $L_e/L_0 = 1/4$, $H_0/A_0 = 2$, $Q = 7.2$. The following values of the material parameters were used: $\dot{\epsilon}/(\sqrt{3}\dot{\gamma}_0) = 2.89 \times 10^{-18}$, $E/s_0 = 9.38$, $s_{ss}/s_0 = 0.79$, $As_0/T =$

Fig. 2. Typical predicted plane strain tension behaviour for a specimen with $B_0/A_0 = 4$, $L_0/B_0 = 2$, $L_e/L_0 = 1/4$, $H_0/A_0 = 2$, $Q = 7.2$, $\xi = 0.01$ and for the following values of the material parameters: $\dot{\epsilon}/(\sqrt{3}\dot{\gamma}_0) = 2.89 \times 10^{-18}$, $E/s_0 = 9.38$, $s_{ss}/s_0 = 0.79$, $A s_0/T = 79.2$, $h/s_0 = 5.15$, $\nu = 0.3$, $\alpha = 0.08$, $N = 2.8$, $C^R/s_0 = 0.132$. Stages a-f correspond to the plots shown in Fig. 3 and Fig. 4.

79.2, $h/s_0 = 5.15$, $\nu = 0.3$, $\alpha = 0.08$, $N = 2.8$, $C^R/s_0 = 0.132$. These values, except for the value of E/s_0 , were primarily used as representative values of the parameters, but are quite reasonable for polycarbonate among other amorphous glassy polymers. In ARGON's [1973] model, the value of E/s_0 is determined uniquely by Poisson's ratio. However, here we consider it to be an independent material parameter, because the constitutive model described in Sec. II cannot account for the small strain viscoelastic behaviour observed in experiments, which results in a nonlinear stress-strain response prior to yielding. Now, as we are mainly interested in large plastic deformations, these viscoelastic effects need not be considered in detail, and we shall simply characterize the behaviour prior to yielding by an appropriate mean value of E (see also WU & VAN DER GIESSEN [1994]). The intensity ξ of the initial imperfection [see eqn (16)] is assumed to be 0.01. We will use these values of the parameters throughout Sec. IV, except where noted otherwise. It should be noted that the gauge section displacement U_g in (17) is determined as the average displacement over the section that was located at $x = B_0$ in the initial configuration.

The four successive stages of the experimental force-elongation curve distinguished by BUISSON and RAVI-CHANDAR [1990] are picked up qualitatively by the simulation (Fig. 2): (I) the elastic response ending at ϵ of about 0.09; (II) a significant force drop, spreading over a strain range from 0.09 to 0.16; (III) a plastic domain with a very small apparent slope, spreading over a strain range from 0.16 to about 0.54; (IV) large plastic flow of the sample with enhanced hardening. The calculation ended when the maximum plastic stretch approached the locking stretch $\sqrt{N}$ of the macromolecular chain network at some point in the specimen.

The process of neck localization and stabilization is also illustrated in Fig. 2, where the thickness-reduction ratio $\kappa = A_N/A_0$ at the minimum section ($x = 0$) is plotted as a function of the elongation $\epsilon = U_g/B_0$. Here we see a rapid decrease in section thickness at the maximum axial force state, and thus represents the onset of localized necking. With further elongation this curve reaches a plateau indicating the stabilization of necking in the minimum section followed by neck propagation along the specimen. In the final stage with enhanced hardening, a somewhat faster decrease in section thickness is found.

The development of the neck is further depicted in Fig. 3 as a series of consecutive deformation states (deformed mesh), which clearly show the various stages of neck ini-

Fig. 3. Deformed meshes under plane strain tension at various deformation stages: (a) $\epsilon = 0.09$, (b) $\epsilon = 0.13$, (c) $\epsilon = 0.16$, (d) $\epsilon = 0.30$, (e) $\epsilon = 0.54$, (f) $\epsilon = 0.60$. All figures are scaled to the same apparent specimen length. The parameters are given in Fig. 2.

tiation (Fig. 3 b), stabilization of neck, and initiation of neck propagation (Fig. 3 c) until locking up (Fig. 3 f). Details of the process of neck propagation are illustrated in Fig. 4, which shows the contours of normalized plastic strain rate $\dot{\bar{\epsilon}}^p$ defined by

$$\dot{\bar{\epsilon}}^p = \frac{\dot{\gamma}^p}{\sqrt{3}} \left(\frac{\dot{U}}{B_0 + U_g} \right)^{-1} = \frac{(1 + \epsilon)}{\sqrt{3}} \frac{\dot{\gamma}^p}{\dot{\epsilon}}.$$

Fig. 4. Contours of normalized plastic strain rate $\dot{\bar{\epsilon}}^p$ under plane strain tension at various deformation stages: (a) $\epsilon = 0.09$, (b) $\epsilon = 0.13$, (c) $\epsilon = 0.16$, (d) $\epsilon = 0.30$, (e) $\epsilon = 0.54$, (f) $\epsilon = 0.60$. All figures are scaled to the same apparent specimen length. The parameters are given in Fig. 2.

In both Fig. 3 and Fig. 4 each state corresponds with states labelled (a) through (f) in the normalized force-elongation curve indicated in Fig. 2. The normalized plastic strain rate distributions indicate where the specimen plastic flow is currently localized.

When the load reaches its maximum, a region of enhanced plastic flow occurs in the center of the specimen. This indicates the initiation of necking (Fig. 4 a), although no neck is visible yet (see profile of the specimen in Fig. 4 a and the deformed mesh in Fig. 3 a). Although the nominal stress decreases during stage II, a region of intense plastic strain rate develops, spreading out over a region of finite extent (Fig. 4 b). This is also demonstrated by the deformed mesh in which we observe that a finite region about the middle of the gauge section ($x = 0$) necks down more or less uniformly (Fig. 3 b). A neck is visible at $\epsilon \approx 0.13$ (Fig. 3 b and Fig. 4 b). In Fig. 4 c the plastic strain rate distribution indicates two crossed, banded regions of enhanced plastic flow. Although these regions do not exhibit all features of a shear band in the sense of a material instability, we shall refer to them as "shear bands" for simplicity. Note that there are two crossed sets of shear bands in the specimen, and the main band orients with the tensile loading axis at an angle of about 54° (rather than 45°). The neck stabilizes when orientation hardening starts to develop in the shear bands. This causes the neighboring material to reach the local shear resistance and initiate substantial plasticity indicating neck propagation (Fig. 4 d-f). This process continues until most of the specimen is well in the plastic, strain hardening regime (Fig. 4 e, f). In this last stage, an apparent hardening also appears in the nominal stress-elongation curve (Fig. 2). During the process of neck propagation, the main shear band clearly indicates the front of the propagating neck. The maximum plastic strain rate always takes place at the symmetry line. Furthermore, the main shear band rotates from 54° to 64° with respect to the tensile axis during neck propagation (Fig. 4 c-f). The reason for this rotation is perhaps the geometry of the specimen used here. When the shear band reaches the right end of the gauge section where the thickness of the specimen is smoothly increasing, the material on the right-hand side of the shear band will force the band to rotate away from the tensile axis.

Quite remarkably, our predicted neck is found to be rather diffuse (see Fig. 3). This is in qualitative agreement with the experimental neck profiles for a typical amorphous polymer like polycarbonate (see e.g. BUISSON & RAVI-CHANDAR [1990]). However, it is noted that very sharp neck profiles have been observed in, for example, polyethylene (see e.g. G'SELL & JONAS [1979]), which is a semicrystalline material. The latter is also the kind of phenomenon studied by HUTCHINSON and NEALE [1983].

At this point it is worthwhile to discuss very briefly the selection of the mesh. Because the material response according to the constitutive model of Sec. II is intrinsically rate-dependent, the mesh sensitivity frequently observed in computational modelling of plastic instability phenomena is not necessarily relevant for the problem under consideration here (see e.g. NEEDLEMAN [1988]). However, the selection of a proper mesh does require attention because the element size defines the minimum possible thickness of the shear band that has been observed. We have used different meshes to simulate neck propagation under plane strain tension. Numerical experiments have shown that the overall response of the specimen, in terms of the overall nominal stress σ and the thickness-reduction ratio κ at the minimum section ($x = 0$) are not sensitive to the mesh. However, to clearly show the front of the propagating neck, a more or less fine mesh is needed. Based on a detailed analysis of the numerical experiments, we decided that a relatively fine mesh with 10×60 elements (10 equally sized elements in y direction, 60 in x direction) would be sufficiently accurate. We will use this mesh, as shown in Fig. 3 a, except where noted otherwise.

IV.2. Effects of initial imperfection

To check the influence of the initial imperfection on necking and neck propagation, we have used different imperfection shapes and sizes in terms of the initial shear strength [cf. eqn (16)]. It was found in all cases that, within the strain-range considered and using the same relative imperfection size (ζ), the overall response is not sensitive to the initial imperfection shape. In fact, we hardly see the effect of the initial imperfection shape on the overall response from the predicted normalized load and thickness reduction. However, the initiation of necking is highly influenced by the amplitude of the initial imperfection. Fig. 5 shows the predicted results by using the same imperfection shape, given by eqn (16), but with different intensities ξ ranging from 0 to 0.02. It is found that decreasing the initial imperfection increases the level of overall elongation at the onset of localization, and that an increasing defect amplitude has the effect of making the descending portion of the normalized load-elongation curve more abrupt (so that the propagation stages begin earlier). After the neck has propagated far away from the central section, the influence of the initial imperfection on the overall responses in terms of σ and κ is no longer distinguishable. Detailed comparisons of deformed meshes using different initial imperfections at various stages of the deformation indicated also that the influence of initial imperfection is very small at large elongations. Furthermore, it should be noted that the specimen we used can be considered as a prismatic specimen having an intrinsic geometric imperfection caused by the grip sections. Therefore, it is not necessary with our specimen to apply an additional initial imperfection for triggering the initiation of necking. As is well-known, in the case of an idealized prismatic specimen (no initial imperfection) with shear free ends there is no evidence of necking and neck propagation.

Fig. 5. Influence of an initial imperfection ξ on the predicted nominal stress response and thickness-reduction ratio under plane strain tension. All other parameters are as in Fig. 2.

IV.3. Effects of material properties

It is generally agreed that the yield and postyield behaviour of glassy polymers exhibit true strain softening (see e.g. HAWARD [1980]). In the BPA model, the effects of softening are described in terms of the evolution equation of the athermal yield strength (2). We study the effects of softening on the initiation of necking and neck propagation by considering different intensities of softening, by taking $s_{ss}/s_0 = 0.79$ and 0.92 , respectively. The associated value of the parameter h , the slope of the yield drop with respect to plastic strain, is adjusted in such a way that the initial slope of softening, $h(1 - s_0/s_{ss})$, remains constant. We also include the limiting case of no intrinsic softening by assuming $s_{ss}/s_0 = 1$.

Fig. 6 a shows the effects of softening on the predicted normalized nominal stress σ . Although the value of the parameter s_{ss}/s_0 determines the extent of intrinsic softening, it is noted that the apparent softening observed in the nominal stress-elongation curve in plane strain tension is partly attributed to the intrinsic material behaviour (*intrinsic softening*), and partly to the occurrence of a reduction of the cross sectional area (*geometric softening*). With the values of the orientation hardening parameters C^R and N used here, the assumption of no intrinsic softening results in no apparent softening in the normalized load-elongation curve too (see Fig. 6 a).

The effect of intrinsic softening on the initiation of necking and neck propagation is more evident from the predicted normalized thickness κ at the minimum section $x = 0$ shown in Fig. 6 b. Although almost the same minimum thickness-reduction ratio $\kappa_{\min} \approx 0.66$ is obtained, the evolution curves of κ are quite different between specimens with different values of intrinsic softening. An increasing intrinsic softening amplitude tends to accelerate the process of neck localization. Detailed comparisons between the plastic strain rate distributions and that in Fig. 4 shows that, although neck propagation begins later, the pattern of necking and neck propagation in the specimen with less intrinsic softening ($s_{ss}/s_0 = 0.92$) is similar to that in Fig. 4. In the case of no intrinsic softening, the thickness-reduction ratio κ is a nearly linear function of applied elongation ϵ . Detailed analysis of the deformed profiles of the specimen at various stages of the deformation process indicates that there is no clear evidence of initiation of necking nor of neck propagation in this limiting case of no intrinsic softening (nor apparent softening). The contours of normalized plastic strain rate at various deformation stages in this case are presented in Fig. 7 and will be discussed later.

The parameters N and C^R govern the orientation hardening through the non-Gaussian network model (6). In Fig. 8, we study the effect of orientation hardening by first using the same value of N ($N = 2.8$) but different values of C^R : $C^R/s_0 = 0.066$, 0.132 , and 0.198 , respectively. Furthermore, we include a limiting case of no orientation hardening by taking $C^R/s_0 = 0$. It is clear from the predicted nominal stress response that a larger value of C^R/s_0 increases the stiffness of the network and therefore increases the orientation hardening. The value of C^R/s_0 is observed to affect the maximum load too. The reason for this is that when the specimen reaches the maximum load state at an applied elongation $\epsilon \approx 0.09$, significant plastic deformation has already occurred at some locations due to the intrinsic inhomogeneity of deformation. If C^R is large, orientation hardening will be already significant at that moment, resulting in a noticeable increase of the maximum load.

The effect of orientation hardening on the initiation of necking and neck propagation is also illustrated in Fig. 8 b in terms of the predicted thickness-reduction ratio κ at the minimum section $x = 0$. It is observed that the larger value of C^R/s_0 , the smaller the minimum normalized thickness $\kappa_{\min}$. It seems that the main effect of orientation

Fig. 6. Influence of the softening parameter s_{ss}/s_0 on the predicted nominal stress response (a) and thickness-reduction ratio (b) under plane strain tension. All other parameters are as in Fig. 2.

hardening on neck localization and neck propagation shown in Fig. 8 b is to shift the normalized thickness-elongation curve vertically without changing its shape.

The predicted deformed meshes at various deformation stages with a large value of $C^R/s_0 = 0.198$ are found to be similar to those shown in Fig. 3. The deformed meshes

Fig. 7. Contours of normalized plastic strain rate $\dot{\epsilon}^p$ in the case without intrinsic softening $s_{ss}/s_0 = 1$ nor apparent softening under plane strain tension at various deformation stages: (a) $\epsilon = 0.09$, (b) $\epsilon = 0.38$, (c) $\epsilon = 0.53$, (d) $\epsilon = 0.60$. All figures are scaled to the same apparent specimen length.

at various deformation stages obtained with $C^R/s_0 = 0$ (i.e. no orientation hardening) are given in Fig. 9. It is found that the initiated neck does not propagate as we observed in the cases with a positive value of C^R/s_0 , but localizes progressively with further elongating (Fig. 9 b, c). The strain is concentrated in the neck area, as is seen from the deformed meshes in Fig. 9 b, c, whereas strains outside the neck region remain almost constant or even slightly decrease. This is also the reason why the predicted nominal stress continues to decrease at large elongations, as shown in Fig. 8 a. Contour plots of plastic strain rate at various stages of the deformation also show no evidence of shear bands in the limiting case of no orientation hardening. In the case of small orientation hardening ($C^R/s_0 = 0.066$), the neck is found to propagate along the specimen but very slowly. All these results indicate that the orientation hardening is the driving force to promote neck propagation along the specimen.

We have also studied the effects of orientation hardening by using the same value of C^R ($C^R/s_0 = 0.132$) but different values of N : $N = 2.8, 4.2$, and 5.6 . It was found that the effect of N on the overall response to plane strain tension of amorphous glassy polymers is not very strong, except for the fact that the limit stretches are reached at different elongation levels.

So far, we have studied the effect of intrinsic softening by using the same values of orientation hardening parameter $C^R/s_0 = 0.132$ and $N = 2.8$ but different values of the intrinsic softening parameter s_{ss}/s_0 ; and the effect of orientation hardening by using the same value of intrinsic softening parameter $s_{ss}/s_0 = 0.79$ but different values of the orientation hardening parameters C^R/s_0 and N . However, it is well-known that both

(a)

(b)

Fig. 8. Influence of the orientation hardening parameter C^R/s_0 on the predicted nominal stress response (a) and thickness-reduction ratio (b) under plane strain tension. All other parameters are as in Fig. 2.

intrinsic softening and geometric softening (reduction of the cross sectional area) affect the softening observed in the load-elongation curve in plane strain tension. Furthermore, the value of C^R/s_0 is observed to affect the apparent softening too. To further determine the effect of intrinsic softening on necking and neck propagation, we will consider

Fig. 9. Deformed meshes for $C^R/s_0 = 0$ at various deformation stages: (a) $\varepsilon = 0.13$, (b) $\varepsilon = 0.19$, (c) $\varepsilon = 0.28$. All figures are scaled to the same apparent specimen length.

here a material without intrinsic softening, but with different values of orientation hardening: $C^R/s_0 = 0.033$, and 0.133 . The predicted overall responses are presented in Fig. 10 in terms of nominal stress σ and the thickness-reduction ratio κ . It is found that, as also demonstrated in Fig. 6 a, in the case of larger orientation hardening ($C^R/s_0 =$

Fig. 10. Influence of the orientation hardening parameter C^R/s_0 on the predicted nominal stress response and thickness-reduction ratio under plane strain tension for a material without intrinsic softening ($s_{ss}/s_0 = 1$). All other parameters are as in Fig. 2.

0.132), the orientation hardening effect suspends the geometric softening effect and excludes the apparent softening in the nominal stress-elongation curve. In this case there is no clear evidence of necking nor of neck propagation along the specimen as demonstrated before; also there is no indication of shear bands (see Fig. 7). In the case of smaller orientation hardening $C^R/s_0 = 0.033$, there is an apparent softening in the nominal stress-elongation curve.

Fig. 11 shows the distributions of normalized plastic strain rate in the specimen with smaller orientation hardening ($C^R/s_0 = 0.033$) at various stages of the deformation. Comparing Fig. 11 with Fig. 4 and Fig. 7, it is seen that, at low elongations, the contours in the case without intrinsic softening but with a small apparent softening in nominal stress-elongation curve (Fig. 11) are similar to those in the case of no intrinsic softening nor apparent softening (Fig. 7); whereas at high elongations, the plastic strain rate distribution in the case without intrinsic softening but with a small apparent softening (Fig. 11) is roughly similar to that in the case with both intrinsic and apparent softening (Fig. 4). At large elongations and with apparent softening, the precise shear band patterns are different when comparing the cases with intrinsic softening (Fig. 4) and without intrinsic softening (Fig. 11). First of all, it is noted that the localization of deformation into what we call shear bands, in the case without intrinsic softening is significantly less pronounced than in the case with intrinsic softening. Furthermore, the main shear band in the case without intrinsic softening is oriented at an angle large than 90° with respect to the loading direction.

Fig. 11. Contours of normalized plastic strain rate $\dot{\epsilon}^p$ in the case of no intrinsic softening but with an apparent softening under plane strain tension at various deformation stages: (a) $\epsilon = 0.10$, (b) $\epsilon = 0.16$, (c) $\epsilon = 0.30$, (d) $\epsilon = 0.43$. All figures are scaled to the same apparent specimen length.

It is well-known that flow in amorphous glassy polymers is a viscous process and the yield stress is strongly strain-rate dependent. Fig. 12 shows the overall responses to plane strain tension deformation at normalized applied strain-rates $\dot{\epsilon}/(\sqrt{3}\dot{\gamma}_0)$ ranging over several orders of magnitude. The increase of the maximum load due to an increase of the strain rate is seen to be small, about 8% for one decade of strain-rate. It seems that the main effect of strain-rate is to shift the nominal stress elongation curve vertically without changing its shape, while the normalized thickness κ is found to be insensitive to the strain rate. The differences in deformed meshes and the distributions of normalized plastic strain rate under different strain-rates are found to be small, so that it is concluded that the initiation of necking and neck propagation are not sensitive to strain-rate within the range considered. It is pertinent to recall here that thermal effects have been neglected in these computations. BOYCE *et al.* [1992] and ARRUDA *et al.* [1995] have explored these effects.

IV.4. Effects of geometry and boundary condition

From the point of view of experiments, detailed analysis of the effects of specimen geometry and boundary conditions on the overall stress strain response and on the necking behaviour is of practical importance. We first study the effect of geometry of the specimen on the overall response in terms of nominal stress σ and thickness-reduction ratio κ . The numerical results with $B_0/A_0 = 4$ and 6.67 but with the same values of L_0/B_0 , L_e/L_0 , H_0/A_0 , and Q are presented in Fig. 13. In the case of $B_0/A_0 = 6.67$ a regular mesh consisting of 16×90 elements is used. We have also analyzed neck localization and propagation in terms of deformed meshes. It is observed that the effect of geometry on the initiation of necking and neck propagation is very small within the considered range of B_0/A_0 .

Fig. 12. Influence of the normalized applied strain-rate $\dot{\epsilon}/(\sqrt{3}\dot{\gamma}_0)$ on the predicted nominal stress response under plane strain tension. All other parameters are as in Fig. 2.

Fig. 13. Influence of the aspect ratio B_0/A_0 of the specimen's gauge section on the predicted nominal stress response and thickness-reduction ratio under plane strain tension. The material parameters are as in Fig. 2.

Fig. 14 shows the predicted overall responses to plane strain tension with different boundary conditions, namely shear free ends and gripped ends. For the specimen with gripped ends, the rate boundary conditions at $x = L_0$ become

$$\dot{u}_x(L_0, y) = \dot{U}, \quad \dot{u}_y(L_0, y) = 0 \quad (20)$$

instead of (14) and the boundary conditions at $x = 0$ are same as in (15), whereas the lateral surfaces of the specimen are also taken to be stress-free.

We have also plotted the deformed meshes and distributions of plastic strain rate at various deformation stages. It is found that with the shape of the specimen considered here, boundary conditions have a negligible effect on necking and neck propagation. In fact, we hardly see the effect of boundary condition on the overall response in terms of nominal stress σ and thickness-reduction ratio κ in Fig. 14. It is obvious that this is not true for a prismatic specimen.

V. DISCUSSION AND CONCLUSION

In this article, a 3-D constitutive model for large strain inelastic deformation of amorphous glassy polymers has been incorporated in finite element computations of plane strain tension, focusing attention on the initiation of necking and neck propagation along the specimen. Results have been given for the overall load-elongation response and the thickness reduction-elongation response to plane strain tension. The effects of initial imperfection, strain softening, orientation hardening, strain-rate, as well as the influences of geometry and boundary conditions have been discussed in detail.

Fig. 14. Influence of the boundary conditions on the predicted nominal stress response and thickness-reduction ratio under plane strain tension. The material parameters are as in Fig. 2.

The predicted results have shown that the constitutive model is able to pick up qualitatively the four successive stages of the experimental force-elongation curve. The experimentally observed initiation of necking and neck propagation have also been predicted well qualitatively.

An important problem in polymer science and technology is to understand what are the driving factors that control the kinetics of necking and neck propagation. By incorporating the 3-D constitutive model of Sec. II in finite element simulations of the plane strain tension of amorphous glassy polymers, the parameter study performed here should be helpful in improving the understanding of the mechanisms of necking and neck propagation. In the simulations of shear band propagation in simple shear tests, WU and VAN DER GIESSEN [1994] concluded that the intrinsic softening is the driving force to promote initiation of the shear band and its propagation in the shear direction, whereas the orientation hardening is the driving force for widening of the shear band. The results presented here lead to concluding that for the adopted constitutive model, the orientation hardening is the driving force to promote neck propagation along the specimen. Is the intrinsic softening the driving force to promote the initiation of necking in plane strain tension too?

Details aside, it is well known that necking in elastoplastic prismatic plane strain bars essentially coincides with a maximum in the load (or nominal stress) versus elongation curve. Even though our specimen is not prismatic, our results support the conclusion that a maximum followed by apparent softening in the nominal stress-elongation curve is necessary and sufficient for the initiation of necking. Our numerical results also demonstrate that intrinsic softening, geometric softening, and orientation hardening determine, in a competitive way, whether or not apparent softening appears. In one of the

cases presented, there was no intrinsic softening, but apparent softening occurred; this supports the conclusion that intrinsic softening is a sufficient condition for necking, but not necessary.

For all material parameter combinations where we found necking, we observed what we called "shear bands" in the propagating necked region. It is of interest to note that these bands were also observed in the absence of intrinsic softening, even though shear bands are commonly associated with a true material instability. However, the localization of deformation in those bands was less intense than when the material showed intrinsic softening, so that the terminology "shear band" becomes somewhat questionable. All these aspects require further study, both experimentally and numerically, and both macroscopically and microscopically.

Concerning the constitutive aspects, it is noted that we use the affine network theory to model orientational hardening. The idea of using an affine network theory to model the stretching of the molecular network assumes that the junction points in the network remain in tact. However, it has been suggested in the literature (see e.g. RAHA & BOWDEN [1972] and BOTTO *et al.* [1987]) that physical entanglements in amorphous polymers are being pulled out during deformation (see also ARRUDA *et al.* [1995]). In terms of our network model this would mean that the number of chains n reduces in the course of the deformation process, whereas the number of links N per chain increases, thus reducing the stiffness of the network. Also it cannot be ruled out that at large deformations, when chains are rotated toward a common axis to such an extent that they become lined up, intermolecular interactions are no longer negligible. Molecular dynamics simulations (GAO & WEINER [1991]) seem to indicate that this may be a significant effect already at relatively small deformation of the molecular chains in the Gaussian regime, and it may be expected to be even more important at the large strain levels in cold drawing considered here. All these constitutive aspects require further study.

A final related point is the effect of thermomechanical coupling on necking and neck propagation in amorphous glassy polymers. Although specimen heating during deformation is not responsible for necking nor a necessary condition for neck propagation in glassy polymers as has been demonstrated by many researchers, it does affect the neck propagation process due to thermal softening of material at higher rates of loading. Recent work by BOYCE *et al.* [1992] indicated that the temperature rise produced in the higher strain rate cases resulted in substantial thermal softening of the material. This greatly increased the post-yield load drop resulting in a much accentuated curvature neck profile. This is consistent with our conclusion that an increasing softening amplitude tends to accelerate the process of neck localization (see Fig. 6 b).

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