Finite viscoplasticity of amorphous glassy polymers in the logarithmic strain space

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ABSTRACT

The paper outlines a new constitutive model and experimental results of rate-dependent finite elastic–plastic behavior of amorphous glassy polymers. In contrast to existing kinematical approaches to finite viscoplasticity of glassy polymers, the formulation proposed is constructed in the logarithmic strain space and related to a six-dimensional plastic metric. Therefore, it a priori avoids difficulties concerning with the uniqueness of a plastic rotation. The constitutive framework consists of three major steps: (i) A geometric pre-processing defines a total and a plastic logarithmic strain measures determined from the current and plastic metrics, respectively. (ii) The constitutive model describes the stresses and the consistent moduli work-conjugate to the logarithmic strain measures in an analogous structure to the geometrically linear theory. (iii) A geometric post-processing maps the stresses and the algorithmic tangent moduli computed in the logarithmic strain space to their nominal, material or spatial counterparts in the finite deformation space. The analogy between the formulation of finite plasticity in the logarithmic strain space and the geometrically linear theory of plasticity makes this framework very attractive, in particular regarding the algorithmic implementation. The flow rule for viscoplastic strains in the logarithmic strain space is adopted from the celebrated double-kink theory. The post-yield kinematic hardening is modeled by different network models. Here, we compare the response of the eight chain model with the newly proposed non-affine micro-sphere model. Apart from the constitutive model, experimental results obtained from both the homogeneous compression and inhomogeneous tension tests on polycarbonate are presented. Besides the load–displacement data acquired from inhomogeneous experiments, quantitative three-dimensional optical measurements of the surface strain fields are carried out. With regard to these experimental data, the excellent predictive quality of the theory proposed is demonstrated by means of representative numerical simulations.

1. Introduction

Amorphous glassy polymers have been widely employed in various practical application areas that cover automotive and construction industry, electronics, optical devices and medical technology, to mention a few. The broad spectrum of application is due to their good processing features, high energy absorption capacity under impact loadings, lower weight relative to glass and excellent optical properties. The geometry of the products used in the above mentioned practical applications is generally three-dimensional and has varying aspect ratio and dimensional scales. Apart from the geometrical challenge, amorphous glassy polymers exhibit rate-dependent finite elastic–plastic material behavior. The elasto-viscoplastic response stems from the inherent disordered micro-structure of the material that is formed by linear polymer chains existing in the
“frozen-in” state. In contrast to elastomers or thermosets, they are generally not cross-linked by chemical bonds but their network structure is rather formed by physical junctions, the so-called entanglements. This intrinsic micro-structure brings along the rate and temperature effects prevailing in the material behavior. The finite elasto-viscoplastic behavior is not specific only to tough polymers but is also observed in brittle polymers on a much smaller scale, especially in the course of crazing. For this reason, both a sound three-dimensional constitutive model accounting for the complicated material behavior and the associated effective numerical algorithm for finite element simulations are of great importance.

1.1. Mechanical behavior of amorphous glassy polymers

Probably, the most illustrative example for the finite elasto-viscoplastic behavior of ductile glassy polymers is the so-called cold drawing process. Fig. 1 depicts the tensile load–displacement curve of a dumbbell-shaped polycarbonate (Makrolon 2607) test piece (ISO 527-Type 1B) undergoing cold drawing. The experiment was conducted on a MTS servohydraulic uniaxial testing machine at a constant cross-head speed \( u = 2 \text{ mm/min} \) and room temperature. The representative stages of the deformation are labeled from (a) to (h) on both the load–displacement diagram and the snapshots of the deformed specimen in Fig. 1. Combination of the load–displacement diagram and the associated images shows the initiation, stabilization and propagation of the neck. Apart from these images, the quantitative principal stretch contours corresponding to the stages (a)–(f) of the experiment are presented in Fig. 2. The contours were obtained by post-processing the recognized part of each associated image whose periphery is highlighted with the solid line in Fig. 2. The commercial software ARAMIS, which is based on the optical measuring technique, the so-called grating method, was used to capture the three-dimensional strain field evolving on the surface of the dumbbell-shaped specimens during deformation. Further details concerning the preparation of specimens and the procedure followed for inhomogeneous strain field measurements are outlined in Section 4.

In Fig. 1, the initial linearly elastic part of the load–displacement curve bounded by the level (a) falls into the range of small deformations. In the succeeding interval, between the stages (a) and (b), the curve gradually becomes non-linear and exhibits viscoelastic charateristics as shown in Fig. 1. At these stages of the extension, the strain field along the specimen is measured to be uniform, see Fig. 2a and b. The highest load level (b) attained at the end of the non-linear viscoelastic part is generally called the macro-yield point. Any unloading below this point does not result in significant hystereses or permanent strains, see Lu and Ravi-Chandar (1999). It has been shown that the pre-yield viscoelastic behavior is essential to elucidate the non-linear unloading and creep response of the material. For more detailed discussions concerning the phenomenon, the reader is referred to the recent works of Hasan and Boyce (1995) and Anand and Ames (2006). Further extension beyond the yield point (b) leads to inelastic strain localization regions that generally appear in the form of micro shear bands causing a softening in the load–displacement response, see Tomita et al. (1997) and Lu and Ravi-Chandar (1999). These bands then
(b) and (d) initiating a macroscopic plastic localization zone, commonly called necking, compare Fig. 1d and Fig. 2d. The contour plot in Fig. 2c corresponding to an intermediate step during the process of neck stabilization clearly exhibits the nature of this process. As depicted in Fig. 1, the thickness of the neck reaches an almost stationary state and stabilizes around the lowest post-yield load level at the stage (d). This is the point where the chains in the active necking zone start plastically to align along the extension direction. The alignment of the molecules results in the so-called strain hardening and causes the neck front to propagate through the test piece at an almost constant load level between the stages (d) and (h). This process is commonly called cold drawing and yields a highly anisotropic deformed state as a result of large inelastic alignment of chains. During this process, the contour plots corresponding to the stages (d)–(f) show some further extension in the already plasticized regions. This is also reflected in the gradual hardening in the load–displacement diagram, albeit its very small value. As the neck shoulders reach the grip zone about point (h), the curve starts to stiffen again and climbs up till the ultimate failure.

In the above-described cold drawing experiment, as the contour plots in Fig. 2 clearly show, beyond the macroscopic yield point (b) the stress/strain field along the specimen is not homogeneous anymore. Besides, the rate of deformation at different material points considerably differs from each other. Since the material response is rate-dependent, any stress–strain relation obtained from such type of experiment without special measuring techniques equipped with specific control devices would not reflect the true local material response, see for example Hope (1980), G’Sell and Jonas (1979) and G’Sell et al. (1992). Owing to the high computational cost, there have been few studies that directly employed uneven field measurements on the surface of the tensile specimen for identifying material parameters of models. In the work of Tomita et al. (1997), the nominal stress measurements at distinct cross-sections of a tensile specimen undergoing highly inhomogeneous deformation are successfully used to identify the material parameters in a hybrid way. In order to circumvent the difficulties associated with the non-homogeneous strain state in tensile experiments, uniaxial and plane strain compression experiments have been carried out to investigate the local stress–strain response. In the compressive uniaxial and plane strain tests a macroscopically homogeneous strain state can be achieved provided that the friction between the specimen and platens is eliminated by the use of an appropriate lubrication technique. For instance, Raha and Bowden (1972) and Bowden and Raha (1970) reported the results of plane strain compression tests on polymethylmethacrylate (PMMA) and polystyrene (PS). The uniaxial and plane strain compression stress–strain data of PMMA and PC up to the true strain value \( \ln \frac{\lambda}{C_0} \) have been presented in Arruda and Boyce (1993a) and Boyce et al. (1994). I nFig. 6b, the true stress–true strain response of polycarbonate under uniaxial and plane strain compression is depicted. As can be noticed immediately, the local stress–strain response exhibits a true strain softening followed by strain hardening at large deformations. The true strain softening is believed to be the result of localized shear band formation accompanied by the evolution of local free-volume, see Argon (1973), Hasan et al. (1993), Hasan and Boyce (1995), and Anand and Gurtin (2003). It has also been observed in Fig. 6b that the yield stress in glassy polymers exhibits both the deformation state and the pressure dependency (Spitzig and Richmond, 1979).
1.2. Constitutive approaches to modeling of glassy polymers

During the transition from a rubbery to a glassy state the random micro-structure of the material is generally conserved, see Treloar (1975). The mobility of the chains, however, is greatly affected by a decrease in temperature. At temperatures well below the glass transition temperature, the mobility of the molecules declines substantially and they exist in a “frozen-in” state. As commonly accepted, two types of physical resistance govern the energy barrier that must be overcome to yield the material and to deform it up to large plastic strains. These are associated with the intermolecular and intramolecular mechanisms, respectively. The plastic flow of glassy polymers is a thermally activated, statistical process whose rate is proportional to the celebrated Boltzmann factor \(\exp(-\Delta G/k\theta)\), where \(\Delta G\), \(k\), \(\theta\) are the energy barrier to be surmounted, the Boltzmann constant, and the absolute temperature, respectively. To achieve the macroscopic yielding, the stress state in the material must be brought to a level at which the necessary thermal energy level for the segment rotation can be attained. This barrier is proved to be closely related to the \textit{intermolecular resistance}, and therefore depends on the pressure, which increases the degree of packing in the material micro-structure. After yielding the material flows and molecules align in the flow direction. During the orientation of chains, the conformational entropy of chains decreases. Similar to the elasticity of rubbery polymers, finite plastic deformations accompanied by strain hardening can only be attained by overcoming the \textit{entropic resistance}, see Haward and Thackray (1968), Rider and Hargreaves (1969) and Argon (1973) among others.

Early theories on glassy polymers, e.g. Marshall and Thompson (1954), attempted to account for the plastic deformation through an increase in chain mobility due to either a deformation induced dissipative heating leading higher temperature or a deformation-induced increase in \textit{free volume} providing more room for the motion. Although these factors facilitate the plastic flow below the glass transition temperature, they cannot be justified as the sole reasons yielding the active motion of molecules, see for instance (Vincent, 1960). Owing to the above arguments, first, visco-elasticity theories have been employed for the description of the phenomena. These theories, being essentially based on Eyring-type (Eyring, 1936) rate equations, are restricted to limited range of temperature and deformation rates. Besides, the physical significance of the phenomenological parameters appearing in the theory remains dubious, see Bowden (1973) and Crist (1997) for a review. These theories have been followed by physically based plasticity models motivated from the experimentally observed permanent residual deformation remaining after unloading. Probably the most significant molecular theories for the rate-dependent inelastic behavior of amorphous polymers have been proposed by Robertson (1966) and Argon (1973). In the Robertson model, plasticity is attributed to a thermally activated transition of molecular chains from flexed to extended configurations by rotation of its segments. This scenario is based on the overcoming of only the \textit{intra}molecular resistance by externally applied stress. The celebrated \textit{double-kink} theory of Argon (1973) is also based on the thermally activated process but the resistance to the flow is primarily attributed to the \textit{inter}molecular interactions via the so-called wedge disclinations, see Li and Gilman (1970). Compared to the former, the latter yields better agreement with the experiments conducted at temperatures well below the glass transition temperature \(\theta_g\). This indicates the importance of intermolecular interactions in the yield mechanism of glassy polymers. On the other hand, the former has been shown to be relatively better at temperatures close to \(\theta_g\), see Argon and Bessonov (1977).

Over the past decades, considerable effort was made to develop three-dimensional constitutive models that account for the finite viscoplastic behavior of glassy polymers. The pioneering works of Boyce, Argon, Parks and co-workers (Boyce et al., 1988; Arruda and Boyce, 1993b; Arruda et al., 1995; Hasan and Boyce, 1995) have been followed, for instance, by Wu and van der Giessen (1993, 1994, 1995), Tomita and Tanaka (1995), Govaert et al. (2000), Anand and Gurtin (2003), among others. The molecular double-kink theory (Argon, 1973) was extended to the three-dimensional formulation by Boyce et al. (1988) where they also incorporated the strain softening by a phenomenological evolution equation for the athermal shear strength. In this work, they applied the double-kink theory to the rate-dependent evolution of finite plastic flow. Kinematics of the plastic deformation is based on the multiplicative split of the deformation gradient into elastic and plastic parts. The immediate outgrowth of this multiplicative split is the hypothetical intermediate configuration. However, in contrast to metals, the rotation is not unique and not well understood in the case of amorphous materials. Therefore, in this context one needs to make an additional assumption concerning the rotation tensor or the plastic spin. Boyce et al. (1989) suggested the elastic part of the deformation gradient to be symmetric. For modeling the strain hardening in the post-yield regime, the entropic network models borrowed from the statistical rubber elasticity theories have been employed. As material temperature is increased above its glass transition temperature without any restraint, it is observed to regain its original shape as well as isotropic molecular structure, see Haward and Mann (1964) and Haward et al. (1971). Therefore, the recovery of the original shape at \(\theta > \theta_g\) provides an evidence for the existence of internal forces, commonly referred to as back stresses at \(\theta < \theta_g\). These may be considered as external forces at \(\theta > \theta_g\) required to keep the material in the deformed state. Moreover, the existence of memory effect necessitates an sparsely connected network structure. In the case of linear glassy polymers, this network structure is provided by entanglements. Owing to the similarity between rubber-like and plastic post-yield responses, as originally suggested by Haward and Thackray (1968), the post-yield strain hardening response was conventionally modeled by the network models proposed in James and Guth (1943), Wang and Guth (1952), Arruda and Boyce (1993b), Wu and van der Giessen (1993), and Tomita et al. (1997).
1.3. Modeling of glassy polymers in the logarithmic strain space

In this contribution, we develop a new finite elasto-viscoplastic model for ductile polymers, in particular polycarbonate, under isothermal conditions at temperatures well below the glass transition temperature $\theta_g$. The key ingredient is the kinematical framework of finite elasto-viscoplasticity adopted from the recently proposed approach by Miehe et al. (2002a). This framework exploits the ideas of the so-called additive metric plasticity similar to the geometrically linear theory of elasto-plasticity. The constitutive framework is constructed in the logarithmic strain space where the elastic part $\varepsilon^e$ of the Lagrangian Hencky strain $\varepsilon := \ln(\mathbf{C})/2$ is defined as $\varepsilon^p := \varepsilon^e - \ln(\mathbf{G}^p)/2 = \varepsilon^e - \varepsilon^C$ where $\mathbf{C} := \mathbf{F}^\top \mathbf{F}$ denotes the right Cauchy–Green tensor. This additive form allows us to formulate finite plasticity in a framework analogous to the geometrically linear theory which in turn leads to a very attractive algorithmic setting. Within this framework the evolution of viscoplastic strains $\varepsilon^p$ is adopted from the celebrated double-kink model of Argon (1973). As conventionally accepted in the literature, the kinematical hardening mechanism due to the plastic alignment of the chains may be modeled by the network models of rubber elasticity. Most models in the literature use the eight-chain model of Arruda and Boyce (1993b). We here also incorporate the recently proposed non-affine micro-sphere model of Miehe et al. (2004). The modeling capacity of the proposed approach is then assessed by comparing the simulation results with the experimental data. For that purpose we carried out macroscopically homogeneous uniaxial and plane strain compression experiments on PC specimens under isothermal conditions. These data are then used to identify the limited material parameters. The performance of the model with the identified material parameters is tested in a three-dimensional finite element simulation of the cold drawing experiment described in Figs. 1 and 2. The comparison includes not only the load–displacement diagram but also three-dimensional strain fields. Comparison of the simulations with experimental results indicate the outstanding quantitative modeling capability of the proposed approach.

The paper is organized as follows. Section 2 briefly outlines the additive kinematic approach to finite inelasticity in the logarithmic strain space and points out the model-independent modular algorithmic structure. Section 3 is devoted to the elasto-viscoplastic constitutive model in the logarithmic strain space and the details of its algorithmic implementation. In Section 4, representative numerical examples illustrating the modeling capabilities of the proposed approach in comparison with the experimental results obtained from the homogenous and non-homogeneous tests are presented.

2. Additive finite plasticity in the logarithmic strain space

Despite the intensive work carried out over the last four decades, the development of a canonical kinematic framework for finite elastoplasticity is still a topic of active research. An exhaustive review of the existing literature on kinematics of finite plasticity is not aimed here but only a few key references will be addressed. For a comprehensive review, the reader is referred to the critical state-of-art manuscripts by Naghdi (1990) and Xiao et al. (2006), among others. Apart from the rate formulations (hypoelasticity), the kinematical approaches to finite plasticity may be roughly classified into two main categories: (a) The formulations based on the multiplicative decomposition of the deformation gradient into the elastic and inelastic parts, i.e. $\mathbf{F} = \mathbf{F}^e \mathbf{F}^p$. (b) The framework constructed on the notion of an additional primitive Lagrangean plastic strain $\mathbf{E}^p$. The former has been motivated from the micromechanical plasticity theory of crystalline materials and applied also to the phenomenological framework of plasticity. The multiplicative split of the deformation gradient, commonly referred to as the Kröner–Lee decomposition, can be traced back to the seminal works of Kröner (1960), Lee (1969) and Mandel (1972). The latter is based on the introduction of the Lagrangean plastic deformation measure $\mathbf{E}^p$ as a primitive variable proposed by Green and Naghdi (1965). This framework, the so-called Green–Naghdi theory, has been further extended by Miehe (1998a,b) based on the notion of the evolving reference plastic metric $\mathbf{G}^p$. Motivating from the notion of Lagrangean plastic metric, an additive framework for the finite plasticity has been recently proposed within a framework of the logarithmic strain space by Miehe et al. (2002a), Papadopoulos and Lu (1998, 2001), and Miehe and Apel (2004). Results of the additive finite plasticity in the logarithmic strain space were compared in Miehe et al. (2002a) with results obtained from classical multiplicative plasticity for both isotropic and anisotropic materials. This comparative study indicates the closeness of the results obtained by the distinct formulations for a broad range of boundary value problems considered. The similarity between the formulation of finite plasticity in the logarithmic strain space and the geometrically linear theory of plasticity makes this formulation highly attractive, especially with regard to the algorithmic implementation.

The kinematic setting of almost all of the proposed approaches to finite viscoplasticity of glassy polymers make use of the Kröner–Lee multiplicative decomposition of the deformation gradient. The immediate outcome of this approach is a stress-free relaxed intermediate configuration which is physically well-justified in the case of crystal plasticity. In the case of non-crystalline materials, however, some additional assumptions for the properties of the elastic part of the deformation gradient (Boyce et al., 1988) or for the plastic spin (Anand and Gurtin, 2003) are required. Being distinct from the former, we here extend the recently proposed alternative additive kinematical approach in the logarithmic strain space by Miehe et al. (2002a) to the finite viscoplasticity of glassy polymers. This framework a priori avoids the difficulties and assumptions associated with the fictitious intermediate configuration and serves as a key advantageous kinematical setting allowing an efficient algorithmic formulation in the six-dimensional symmetric space.
2.1. Additive kinematic approach based on logarithmic strains

Being consistent with the Kröner–Lee decomposition, a multiplicatively defined objective strain variable of the form

\[ \varepsilon_m^e := f_m(F^0TGF^0) \]  

(1)

enters an elastic energy storage function of the constitutive model. The convected current metric \( C := F^TgF \) is a function of the deformation \( F \) of the material, see Fig. 3a. The plastic map \( F^p \) is considered as an internal variable that describes the plastic flow through the crystal by multiple shearing on crystallographic slip planes in crystalline materials. For isotropic as well as anisotropic materials with preferred structural directors which deform with the material it can be shown that the plastic map enters stored energy functions through the metric \( G^p := F^{pT}GF^p \), see Fig. 3b. This justifies a framework of finite plasticity based on a plastic metric \( G^p \) that is a priori considered as an internal variable. A particular additive dependence of the Lagrangian elastic strain variable on \( C \) and \( G^p \) is provided as

\[ \varepsilon_m^e := f_m(C) - f_m(G^p) \]  

(2)

Here, the tensor-valued isotropic tensor function \( f_m \) characterizes the Seth-Hill family of generalized strain measures defined by

\[ f_m(A) = \begin{cases} \frac{1}{m} (A^{m/2} - 1) & \text{if } m \neq 0, \\ \frac{1}{2} \ln A & \text{if } m = 0, \end{cases} \]  

(3)

where all \( m \in \mathbb{R} \) and \( A \in \text{Sym}(3) \). The specific choices of \( m = 0, 1, 2 \) defines the Hencky strain, the Biot strain and the Green strain, respectively, in the Lagrangian geometric setting of finite elasticity. For the Green–Lagrangian strains with \( m = 2 \), it is readily observed that the basic invariants of (1) coincide with those of (2) when the latter are computed with respect to the plastic metric. This already makes clear for an isotropic integrity basis that the use of the Lagrangian elastic strain measure (2) is in general consistent with the approach (1) only if the energy storage function depends on \( \varepsilon_m^e \) and \( G^p \). However, choosing \( m = 0 \) in (1) and (2), we observe \( \varepsilon_m^e = \varepsilon_m^0 \) for the special case of coaxial total and plastic deformations where \( C \) and \( G^p \) commute and the plastic map is identified by \( F^p = G^{01/2} \). In this case, the logarithmic Lagrangian elastic strain measure defined by

\[ \varepsilon^e := \frac{1}{2} \ln C - \varepsilon^p \]  

(4)

brings the additive split (2) at least closer to the multiplicative form (1). The logarithmic plastic strain \( \varepsilon^p := (1/2) \ln G^p \) defined in (4) with \( G^p(t_0) = G \) may be considered as the internal variable that enters the constitutive formulation.

2.2. Modular structure of the constitutive equations

The additive decomposition of the total strains into elastic and plastic parts is a typical feature of the geometrically linear theory of plasticity. Thus the form (4) provides a natural basis for a material-independent extension of constitutive structures from the geometrically linear theory to the nonlinear theory at finite strains. The point of departure for this extension is an a priori six-dimensional approach to finite plasticity based on the notion of a plastic metric. Within this general framework, we consider three modules which define a class of finite plasticity models consistent with (4):

- **Geometric pre-processor** defines the total and plastic logarithmic strain measures, which are obtained from the current and plastic metric, respectively.
- **Constitutive model** describes the constitutive equations for elasto-viscoplasticity in the logarithmic strain space in a structure identical to geometrically linear theory.

![Fig. 3](image)

**Fig. 3.** Definition of metric and stress tensors as mappings. (a) Current metric: \( g \), in Lagrangian configuration \( C := F^TgF \). (b) Plastic metric: \( G^p \), in Eulerian configuration \( c^p := F^{-1}G^pF \). (c) Nominal stress: \( P \), Eulerian Kirchhoff stress \( \tau := PF^T \), Lagrangian second Piola–Kirchhoff stress \( S := F^{-1}P \).
Geometric post-processor maps the objects obtained in the logarithmic strain space to their nominal, Lagrangean or Eulerian counterparts.

The attractive feature of the above-outlined modular structure of finite plasticity is the possibility to adopt known constitutive models of the infinitesimal theory as a module in the logarithmic space. We apply this framework to a model of rate-dependent elastoplasticity for modeling of glassy polymers by taking into account the orientation hardening, which can be modeled by the network models of rubber elasticity, such as the eight-chain model of Arruda and Boyce (1993b) and the recently proposed non-affine micro-sphere model of Miehe et al. (2004).

2.2.1. Geometric pre-processing of the logarithmic strain space

A key point in constructing a framework of finite plasticity is the definition of an elastic strain measure $\mathbf{e}$. This measure enters as a variable the constitutive function that describes the macroscopic elastic energy storage. We assume this strain measure to be a function of the above-introduced Lagrangean current and plastic metric tensors, i.e.

$$\mathbf{e}^e = \mathbf{e}^e(\mathbf{C}, \mathbf{G}^p).$$

The elastic strain can be conceptually defined based on the notion of additive form as

$$\mathbf{e}^e := \mathbf{e} - \mathbf{e}^p$$

being consistent with (4) in terms of the logarithmic Lagrangean total and plastic strains

$$\mathbf{e} := \frac{1}{2} \ln \mathbf{C} \quad \text{and} \quad \mathbf{e}^p = \frac{1}{2} \ln \mathbf{G}^p,$$

respectively. The logarithmic tensor function $\mathbf{f}_p$, maps the multiplicative characteristics of large-strain elasto-plasticity to the additive structure of the geometrically linear theory. In particular, we observe the relationship

$$J^p := \sqrt{\det[\mathbf{G}^p]} = \exp[\text{tr}[\mathbf{e}^p]]$$

for the plastic jacobian that governs the change of volume due to plastic deformation. Recall that the plastic incompressibility condition demands

$$\det[\mathbf{G}^p] = 1 \iff \text{tr}[\mathbf{e}^p] = 0.$$

The incompressibility constraint on the plastic metric $\mathbf{G}^p$ in the context of an isochoric plastic flow is described by the additive constraint on the trace of the logarithmic plastic strain $\mathbf{e}^p$. As already mentioned above this is the key property that motivates the choice of the logarithmic strain measures (7). Owing to the one-to-one relationship between $\mathbf{G}^p$ and $\mathbf{e}^p$ in (7)1, we may consider the logarithmic plastic strain measure $\mathbf{e}^p$ as an internal variable alternative to $\mathbf{G}^p$. The evolution of $\mathbf{e}^p$ is then exclusively defined in the constitutive box associated with the logarithmic strain space defined below.

The derivation of the transformation tensors of the logarithmic strain space is a purely geometrical operation that is based on the stress power

$$\mathcal{P}(t) := \mathcal{P}(t) : \mathbf{F}(t)$$

defined per unit reference volume of the material. The power expression in (10) is represented in terms of the non-symmetric nominal stress tensor $\mathbf{P}$ considered in Fig. 3c. This tensor is said to be work-conjugate to the rate $\mathbf{F}$ of deformation. The non-symmetric tensors $\mathbf{P}$ and $\mathbf{F}$ are considered as the work pair of dual external variables of the local elastic–plastic material element. The logarithmic strain measure $\mathbf{e}$ defined in (7)1 is a function of the current metric $\mathbf{C}$, which in turn depends also on the deformation $\mathbf{F}$ and the Eulerian standard metric $\mathbf{g}$ due to the pull-back operation on $\mathbf{g}$ illustrated in Fig. 3a. The key intrinsic feature of the subsequent treatment is the computation of the sensitivity of this strain measure with respect to a change of the deformation. To this end, we introduce the relationships

$$\dot{\mathbf{e}} = \mathcal{Q} : \mathbf{F} \quad \text{and} \quad \dot{\mathcal{Q}} = \mathcal{L} : \mathbf{F}$$

in terms of the fourth and sixth order nominal transformation tensors defined by

$$\mathcal{Q} := \mathcal{Q}_f \mathbf{e} \quad \text{and} \quad \mathcal{L} := \mathcal{L}_f \mathbf{e},$$

respectively. These transformation tensors play a central role in the succeeding treatment. Insertion of the inverse form of (11)1 into (10) leads us to an alternative description of the stress power

$$\mathcal{P}(t) := \mathbf{\alpha}(t) : \mathbf{e}(t),$$

where $\mathbf{\alpha} := \mathbf{P}^{-1}$ stands for the Lagrangean stress tensor work-conjugate to the logarithmic strain measure $\mathbf{e}$. The symmetric Lagrangean tensors $\mathbf{\sigma}$ and $\mathbf{e}$ provide a convenient pair of dual external variables of the local material element associated with the logarithmic strain space. It is worth remarking on that for an isotropic hyperelastic material, the stress tensor $\mathbf{\sigma} := \mathcal{Q}W(\mathbf{e})$ coincides with the so-called rotated stress tensor obtained by the pull-back of the Kirchhoff stress tensor $\mathbf{\tau}$ with
the rotational part \( \mathbf{R} \) of the deformation gradient \( \mathbf{F} \), i.e., \( \sigma = \mathbf{R}^T \mathbf{r} \mathbf{R} \). For a different interpretation and a derivation of the rotated stress tensor \( \sigma \), the reader is referred to Simo and Marsden (1984).

2.2.2. Constitutive model in the logarithmic strain space

Now we consider a constitutive model of rate-dependent elastoplasticity that is exclusively restricted to the logarithmic strain space. This model is considered as a constitutive box, its input being given by the logarithmic strain measure \( \varepsilon \) and a set \( \mathcal{S} := \{ \mathcal{E}^p, \ldots \} \) of internal variables consisting of the logarithmic plastic strain tensor \( \mathcal{E}^p \) and some additional internal variables. What comes out of the constitutive box is the current stress \( \sigma \) dual to the logarithmic strain \( \varepsilon \) and the associated algorithmic elastic–plastic tangent moduli \( \mathcal{E}_{\text{algo}} \):

\[
\{ \varepsilon, \mathcal{S} \} \Rightarrow \text{MODEL} \Rightarrow \{ \sigma, \mathcal{E}_{\text{algo}} \}.
\]

The attractive feature of the constitutive model is that it can preserve the structure of plasticity model of geometrically linear theory and thus the model can adopt standard constitutive structures of the small strain theory. The details of the specific constitutive model for viscoplasticity of glassy polymers are elucidated in Section 3.

2.2.3. Geometric post–processing of nominal stresses and moduli

Once the stresses and consistent tangent moduli in the logarithmic strain space have been obtained from the constitutive model in (14), we map them to the nominal stresses and nominal moduli based on the straight forward application of the transformation rules introduced in Section 2.2.1. Taking into account (13), (12), and (11), we obtain

\[
P = \sigma : \mathcal{Q} \quad \text{and} \quad \mathcal{A}_{\text{algo}} = \mathcal{Q}^T : \mathcal{E}_{\text{algo}} : \mathcal{Q} + \sigma : \mathcal{L}.
\]

in terms of the transformation tensors introduced in (12) with respect to the rate of deformation. Clearly, the recovery of the plastic metric from the logarithmic strain space is obtained by the exponential map \( \mathcal{G}^p = \exp[2\mathcal{E}^p] \) as an inverse to the logarithmic map (7).

Equations (7), (14), and (15) represent the three key steps of the modular constitutive structure of finite plasticity in the continuous setting.

2.2.4. Geometric post-processing of Lagrangean and Eulerian objects

The symmetric Lagrangean stresses \( \mathbf{S} := \mathbf{F}^{-1} \mathbf{P} \) considered in Fig. 3c and their associated elasto-plastic tangent moduli \( \mathcal{C}_{\text{algo}} \) are obtained analogously to the above derivation of the nominal tensors. We get the representations

\[
\mathbf{S} = \sigma : \mathcal{Q}_L \quad \text{and} \quad \mathcal{C}_{\text{algo}} = \mathcal{Q}_L^T : \mathcal{E}_{\text{algo}} : \mathcal{Q}_L + \sigma : \mathcal{L}_L
\]

in terms of the fourth- and sixth-order Lagrangean transformation tensors \( \mathcal{Q}_L \) and \( \mathcal{L}_L \), respectively. They are defined as the derivatives of the logarithmic strain measure with respect to the convected current metric \( \mathbf{C} \).

\[
\mathcal{Q}_L := 2\mathcal{E}_L \quad \text{and} \quad \mathcal{L}_L := 4\mathcal{E}_L^2 \mathcal{E}.
\]

The Lagrangean consistent tangent moduli \( \mathcal{C}_{\text{algo}} \) govern the sensitivity of the symmetric Piola–Kirchhoff stress with respect to the Lagrangean rate \( \dot{\mathbf{C}} \) of deformation by

\[
\dot{\mathbf{S}} = \mathcal{C}_{\text{algo}} : \frac{1}{2} \dot{\mathbf{C}}.
\]

For the sake of completeness, we also consider the Eulerian–Kirchoff stresses \( \mathbf{r} := \mathbf{P} \dot{\mathbf{F}} \) and their associated tangent moduli \( \mathcal{C}_{\text{algo}} \). Being analogous to (15) and (16), we get

\[
\mathbf{r} = \sigma : \mathcal{Q}_E \quad \text{and} \quad \mathcal{C}_{\text{algo}} = \mathbf{Q}_E^T : \mathcal{E}_{\text{algo}} : \mathbf{Q}_E + \sigma : \mathcal{L}_E.
\]

in terms of the Eulerian transformation tensors \( \mathcal{Q}_E \) and \( \mathcal{L}_E \) that are defined as derivatives of the logarithmic strain measure with respect to the Eulerian standard metric \( \mathbf{g} \) in the form

\[
\mathcal{Q}_E := 2\mathcal{E}_E \quad \text{and} \quad \mathcal{L}_E := 4\mathcal{E}_E^2 \mathcal{E}.
\]

The Eulerian tangent \( \mathcal{C}_{\text{algo}} \) governs the objective rate equation for the Lie derivative \( \dot{\mathbf{r}} = \mathbf{F} \dot{\mathbf{S}} \dot{\mathbf{F}}^T \) of the Kirchhoff stresses

\[
\dot{\mathbf{r}} = \mathcal{C}_{\text{algo}} : \frac{1}{2} \dot{\mathbf{g}}.
\]

For the explicit forms of the transformation tensors of the stresses and tangent in the logarithmic strain space to their nominal, Lagrangian or Eulerian counterparts we refer to Miehe and Lambrecht (2001).

3. Constitutive model for viscoplasticity of glassy polymers

In the preceding section, the modular overall kinematic framework of the proposed model was outlined in the logarithmic strain space. In this section, we first introduce the overall constitutive equations and then specify the constitutive functions in the logarithmic strain space analogous to the geometrically linear theory.
3.1. Overall constitutive structure

The state of the material at a local material point is assumed to be described by the total Hencky strain $\varepsilon$ and the plastic strain $\varepsilon^p$ that have been introduced in (7). The selected thermomechanical potential, the Helmholtz free energy, is then formulated in terms of the state variables

$$\psi = \psi(\varepsilon, \varepsilon^p) = \psi^e(\varepsilon - \varepsilon^p) + \psi^p(\varepsilon^p)$$

per unit reference volume. The free energy is additively split into an elastic part and a plastic part. The former represents the stored energy due to the elastic deformations, the latter, on the other hand, describes the transformational energy stored in the plastically deformed regions. This part acts as a potential for back stresses that drive essentially thermal recovery from the plastically deformed state to the undeformed state upon an increase in ambient temperature above the glass transition temperature $T_g$. The total stresses $\sigma$ and the back stresses $\beta$ are then determined directly from the free energy by following the well-known methodology in Coleman and Gurtin (1967)

$$\sigma := c_\psi(\varepsilon - \varepsilon^p) \quad \text{and} \quad \beta := c_\psi(\varepsilon^p),$$

respectivey. With these definitions at hand, we can now express the local dissipation per unit reference volume in the form

$$\mathcal{D} := \sigma^0 : \dot{\varepsilon}^p \geq 0$$

where $\sigma^0 := -c_\psi = \sigma - \beta$ denotes the thermodynamic driving stress tensor conjugate to the plastic strains $\varepsilon^p$. In order to complete the overall constitutive framework what remains to be defined is the evolution rule for the plastic strains $\varepsilon^p$. To this end, we consider a viscoplastic flow rule having the form

$$\dot{\varepsilon}^p := \dot{\gamma}^p \frac{\text{dev}(\sigma^0)}{\text{dev}(\sigma^0)}$$

where $\dot{\gamma}^p \geq 0$ and $\text{dev}(\sigma^0) := \sigma^0 - \frac{1}{3} \text{tr}[\sigma^0] \mathbf{1}$ with $\text{tr}[\bullet] := (\bullet) : \mathbf{1}$. Notice that for the initial value of the plastic strain tensor $\varepsilon^p(t_0) = 0$, the plastic deformation remains volume conserving, i.e. $\text{tr} \varepsilon^p(t) = 0$. This is in accordance with the finite viscoplastic behavior of ductile glassy polymers that undergo plastic deformations chiefly by shear yielding without exhibiting dilative plastic flow, such as crazing. The only restriction dictated by the second law of thermodynamics (24) on the model is the positiveness of the amount of plastic strain rate $\dot{\gamma}^p$. That is, the model is said to be thermodynamically consistent if the viscoplastic evolution rule fulfills the condition $\dot{\gamma}^p \geq 0$. As will be shown in the subsequent part, this requirement is identically satisfied due to the exponential form of the flow rule.

3.2. Specific forms of the constitutive equations

The above-outlined model of viscoplasticity is basically governed by the three constitutive functions: The elastic $\psi^e(\varepsilon - \varepsilon^p)$ and the plastic $\psi^p(\varepsilon^p)$ parts of the free energy, and the viscoplastic flow rule $\dot{\gamma}^p$. In this section, the specific forms of these constitutive functions shall be introduced.

3.2.1. The elastic free energy

As discussed in Section 1.1, the experimental observations presented in Figs. 1 and 6 as well as in the literature indicate that the deformation in the pre-yield branch is limited to small values compared to the plastic strains attained. In spite of the viscoelastic effects leading to a non-linearity prior to the macroscopic yield, we left them off the present formulation. For this reason, linear elasticity in the logarithmic strain space is considered to be sufficient for the current scope. To this end, we choose a quadratic form for the elastic free energy in terms of elastic strains $\varepsilon^e := \varepsilon - \varepsilon^p$

$$\psi^e = \psi^e(\varepsilon - \varepsilon^p) = \frac{K}{2} \text{tr}^2 [\varepsilon - \varepsilon^p] + \mu \text{dev}[\varepsilon - \varepsilon^p] : \text{dev}[\varepsilon - \varepsilon^p],$$

where $K$ and $\mu$ are the bulk and the shear moduli, respectively. This particular form of $\psi^e$ immediately yields the stress expression through (23)

$$\sigma := -p \mathbf{1} + 2 \mu \text{dev}[\varepsilon - \varepsilon^p] \quad \text{with} \quad p := -K \text{tr}[\varepsilon - \varepsilon^p].$$

It is worth noting that the ellipticity of the elastic free energy $\psi^e$ given in (26) is restricted to a certain interval of elastic strains $\varepsilon^e$, see e.g. Miehe and Lambrecht (2001) and Bruhns et al. (2001). For instance, it can be readily shown that the maximum value of the stretch $\lambda$ in a uniaxial test is bounded by $\lambda = \exp[1]$ in the case of incompressible elasticity. For most of glassy polymers undergoing finite deformations well below the glass transition temperature, however, the range of elastic deformations is far below this limit. Therefore, the present formulation at hand does not run any risk of contradicting the ellipticity requirements.

3.2.2. The plastic free energy accounting for the post-yield hardening

The second constitutive function to be specified is the plastic part of the free energy $\psi^p$. It describes the viscoplastic kinematical hardening through the back stresses that have been introduced in (23)$_2$. As originally proposed by Halloward and
Thackray (1968), the form of the plastic free energy has been conventionally adopted from the theory of entropic rubber elasticity based on finite extensibility of the polymer chains. This part essentially models the intramolecular resistance to the plastic flow due to the alignment of the chains in the principal deformation direction. The key physical motivation is due to the celebrated experiment which demonstrates that a plastically deformed glassy polymer test piece recovers its original undeformed shape upon heating above the glass transition temperature, see Haward and Mann (1964) and Boyce and Haward (1997). The thermal energy input activates the plastically stored energy in the material possessing an entangled network structure. For this reason, it is common practice to model the post-yield strain hardening by using network models that provide a bridge between micro and macro deformations through particular kinematical assumptions. To this end, we consider two network models, the eight chain model of Arruda and Boyce (1993b) and the non-affine micro-sphere model of Miehe et al. (2004), see also Miehe and Göktepe (2005) and Göktepe and Miehe (2005) for the extensions to finite rubber inelasticity. In contrast to the affine network models, such as the three chain model of James and Guth (1943) and Wang and Guth (1952), and the affine full network model of Treloar (1946) and Treloar and Riding (1979), these non-affine network models define a single deformation measure for the whole polymer network. The superiority of the non-affine models to the models based on affine kinematics becomes more transparent as the plane strain and biaxial deformation states are considered besides the uniaxial stress state, see Arruda and Boyce (1993a), Wu and van der Giessen (1993), Miehe et al. (2004), Boyce and Arruda (2000), and Markmenn and Verron (2006)) for a review.

The plastic network free energy modeling the post-yield hardening is specified in the non-Gaussian form in terms of the network plastic stretch $\lambda^p = \tilde{\lambda}^p(\varphi^p)$

$$\psi^p = \tilde{\psi}^p(\lambda^p) = \mu_p N_p \left( \lambda^p \varphi^{-1}(\lambda^p) + \ln \frac{\varphi^{-1}(\lambda^p)}{\sinh \varphi^{-1}(\lambda^p)} \right),$$

where $\mu_p, N_p$ are the material parameters standing for the plastic shear modulus and the number of segments in a polymer chain, respectively. The function $\varphi^{-1}$ denotes the inverse of the well-known Langevin function defined by $\varphi(\cdot) := \coth(\cdot) - 1/\cdot$. The parameter $N_p$ controls the limited extensibility range of chains through the relative plastic network stretch defined by $\lambda^p := \lambda^p / \sqrt{N_p}$. For the particular form of $\tilde{\psi}^p$ in (28), the back stresses can be readily computed by (23),

$$\beta := \partial_{\varphi^p} \psi^p(\lambda^p) = \psi^p \partial_{\varphi^p} \lambda^p,$$

where $\psi^p := \partial_{\varphi^p} \tilde{\psi}^p = \mu_p \varphi^p (3N_p - \lambda^p) / (N_p - \lambda^p)$. In the derivation of $\psi^p$, we employed the Padé approximation of the inverse Langevin function $\varphi^{-1}(\lambda^p) \approx \lambda^p (3N_p - \lambda^p) / (N_p - \lambda^p)$ as proposed by Cohen (1991). Before specifying the functional dependency of the plastic network stretch on the plastic strain tensor $\varphi^p$ for the respective network models, we introduce the reference plastic metric in the inverse form of (7)_2

$$G^p := \exp[2\varphi^p] = \sum_{k=1}^3 \lambda^p_{A_k} n^A_k \otimes n^A_k$$

being co-axial to the plastic strain tensor $\varphi^p = \sum_{k=1}^3 \varepsilon^p_{A_k} n^A_k \otimes n^A_k$ with $\varepsilon^p_{A_k} := \ln \lambda^p_{A_k}$.

In the eight chain model, the plastic stretch of a chain extending from the center of a plastically deformed rectangular prism having the edges oriented in the principal plastic directions $n^A_k$ is assumed to be representative for the whole polymer network, see Fig. 4a. Thus, the plastic network stretch of the eight chain model $\lambda^p_{8c}$ is obtained in terms of the first invariant of the reference plastic metric $G^p$

$$\lambda^p_{8c} := \sqrt[3]{\text{tr}[G^p]}.\tag{31}$$

One of the basic ideas proposed in the non-affine micro-sphere model was the introduction of a field of stretch fluctuations $f$ defined on the micro-sphere $\mathcal{S}$ of space orientations, see Fig. 4b. This fluctuation field multiplicatively links the microstretch $\lambda$ of the single chain to the line-stretch $\lambda$ of the continuum in the format $\lambda = \lambda f$. The fluctuation field $f$ was determined.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig4.png}
\caption{Polymer network models employed for modeling the post-yield kinematic hardening. (a) The eight chain model of Arruda and Boyce (1993b) and (b) the non-affine micro-sphere model of Miehe et al. (2004).}
\end{figure}
by a principle of minimum averaged free energy conceptually in line with homogenization concepts for composites, see e.g. Ponte Castañeda and Suquet (1998), Miehe et al. (2002b), and Miehe (2003). The minimization principle is assumed to be constrained by a $m$-root averaging condition, yielding a closed-form result for the non-affine network stretch

$$J_{ms}^P := \left( \frac{1}{|\mathcal{V}|} \int_{\mathcal{V}} (\lambda)^m dA \right)^{1/m} = (\langle \lambda^m \rangle)^{1/m},$$

(32)

where $m > 0$ is considered as an additional material parameter that describes the non-affine stretch characteristics. The affine plastic stretches $\lambda^P$ in the direction of the Lagrangean unit vectors $\mathbf{r}$ are determined by

$$\lambda^P := \sqrt{\mathbf{r} \cdot \mathbf{G}^P \mathbf{r}},$$

(33)

where the orientation of the Lagrangean unit vectors is governed by spherical coordinates $\mathbf{r}(\phi, \theta) = \cos \phi \sin \theta \mathbf{e}_1 + \sin \phi \sin \theta \mathbf{e}_2 + \cos \phi \mathbf{e}_3$ in a fixed standard Cartesian frame $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ with $\phi \in \mathcal{D}_\phi := [0, 2\pi]$ and $\theta \in \mathcal{D}_\theta := [0, \pi]$, see Fig. 4b. Notice that for a special choice of $m = 2$, this model recovers the eight chain model as a special case due to the identity $(\mathbf{r} \otimes \mathbf{r}) = (1/3) \mathbf{1}$.

Having the respective plastic network stretches defined in (31) and (32), we can proceed with the determination of the tensorial part of the back stresses $\partial_s \lambda^P$ introduced in (29). For the eight chain model, we have $\lambda_{ec}^{P2} = (1/3) tr[G^P] = \sum_{i=1}^3 (1/3) \exp[2s_{ik}^P]$. Making use of the result $\partial_s e^P = n^P_k \otimes n^P_l$, we obtain

$$\partial_s \lambda^P_{ec} = \frac{3}{2} \sum_{i=1}^3 \frac{\exp[2s_{ik}^P]}{3 \lambda_{ec}^P} n^P_k \otimes n^P_l = (3 \lambda_{ec}^P)^{-1} G^P$$

(34)

that yields the closed-form expression for the back stresses

$$b_{ec}^P = \tilde{\mu}_{ec}^P (\lambda_{ec}^P) G^P$$

(35)

where $\tilde{\mu}_{ec}^P (\lambda_{ec}^P) := \mu^P (3N_p - \lambda_{ec}^{P2})/(3(N_p - \lambda_{ec}^{P2}))$. In order to compute the explicit form of the back stresses for the micro-sphere model, we determine $\partial_s \lambda^P = \mathbf{r} \otimes (\lambda^P)$ and $\partial_s \lambda_{ms}^P = ((\lambda_{ms}^P)^{1-m}/(\lambda_{ms}^P)^{m-2} \mathbf{r} \otimes \mathbf{r})$. Incorporation of these results in (29) leads us to

$$b_{ms}^P = \tilde{\mu}_{ms}^P (\lambda_{ms}^P) ((\lambda^P)^{m-2} \mathbf{r} \otimes \mathbf{r}) : b^P,$$

(36)

where $\tilde{\mu}_{ms}^P (\lambda_{ms}^P) := \mu^P (3N_p - \lambda_{ms}^{P2})/(2(N_p - \lambda_{ms}^{P2}))$ and $b^P := \partial_s \lambda^P$.

3.2.3. The flow rule based on the double-kink theory

As discussed in Section 1.2, the viscoplastic flow of amorphous glassy polymers is a thermally activated stochastic process the rate of which $\gamma^P$ is conventionally described by the Arrhenius-type equation $\gamma^P = \gamma_s \exp(-\Delta G_s/kT)$ without the Boltzmann factor $\exp(-\Delta G_s/kT)$. In the present model, we conceptually follow the well-accepted double-kink theory of Argon (1973) based on the wedge disclinations, see Fig. 5a. In this approach, the plastic flow is considered as a rotation of small polymer molecule segments from their initial randomly oriented, flexed state to the principal deformation direction. In order to compute the activation energy, the reverse process is modeled by the formation of a kink pair resisted both by intra- and intermolecular oppositions. At temperatures, well below the glass transition temperature, the intermolecular resistance due to the elastic interaction between a disclination loop and neighboring chains governs the major part of the overall activation energy necessary for the formation of a double kink.

The activation energy to be surmounted is determined by subtracting the amount of work $\Delta W$ done by externally applied effective shear stress $\tau$ from the free energy $\Delta F$ stored during formation of a pair of disclination loops in the surrounding medium, see Fig. 5b. The total micro-free energy $\Delta F$ was already computed in Li and Gilman (1970) where they employed

---

Fig. 5. Double-kink theory of Argon (1973). (a) Formation of a molecular double-kink by a pair of wedge disclination loops. (b) Reverse plastic flow mechanism by formation of a pair of kinks in a polymer molecule embedded in a surrounding elastic matrix, see also (Li and Gilman, 1970).
the Volterra’s method (Love, 1944) for the determination of the displacement field. The linear elasticity constitutive equations have then been used for determining the far stress field over the domain. The strain energy could be estimated by integrating the stress field \( \sigma_{xx} \) outside the disclination loop. This yields a free energy \( \Delta F_{\text{int}} = 3 \pi a^3 \mu \omega^2 / (32 (1 - \nu)) \) for a single disclination loop. Apparently, there exists a negative interaction energy due to the integration of the stress field of one disclination loop over another. The interaction energy between two disclination loops having the same strength \( \omega \) and cylinder radius \( a \) gets the form \( \Delta F_{\text{int}} = 9 \pi a^3 \mu \omega^2 / (8 (1 - \nu)z^2) \). The overall free energy stored due to the two wedge disclinations surrounded by the elastic medium with the shear modulus \( \mu \) and the Poisson’s ratio \( \nu \) is then \( \Delta F = 2 \Delta F_{\text{int}} = 3 \pi a^3 \mu \omega^2 / (16 (1 - \nu)) - 9 \pi a^3 \mu \omega^2 / (8 (1 - \nu))(a/\alpha)^5 \). When a pair of disclination loops is formed, the rotation \( \omega \) yields a compressive strain field proportional to \( z(1 - \cos \omega) \). The amount of work done by the externally applied constant shear stress is determined via incompressibility assumption \( \Delta W = \pi a^2 \omega^2 \tau(z/a) \). The amount of the activation free enthalpy can then be expressed by combining these results

\[
\Delta G_f = \Delta F - \Delta W = \frac{3 \pi a^3 \mu \omega^2}{16 (1 - \nu)} - \frac{9 \pi a^3 \mu \omega^2}{8 (1 - \nu)} \left( \frac{\alpha}{z} \right)^5 - \pi a^3 \mu \omega^2 \left( \frac{1}{\mu} \right) \left( \frac{z}{a} \right).
\]

(37)

It can be immediately seen that \( \Delta G_f \) does not contain any extremum in \( \omega \), but in the \( z \) coordinate due to the assumption that intermolecular interactions are dominating compared to the intramolecular ones. Setting the derivative of the activation free enthalpy with respect to the ratio \( z/a \) to zero yields \( (z/a)^* = [45 \mu/(8 \pi (1 - \nu))]^{1/6} \), and its insertion into (37) gives

\[
\Delta G_f' = 3 \mu a^3 \omega^2 \left[ 1 - \left( \frac{\tau}{s_0} \right)^{5/6} \right]
\]

(38)

where the athermal shear strength defined by \( s_0 := 0.077 \mu / (1 - \nu) \). Use of this result in the Arrhenius equation \( \dot{\gamma}^p = \gamma_0 \exp(-\Delta G_f' / kT) \) leads us to the flow rule

\[
\dot{\gamma}^p := \gamma_0 \exp \left[ -\frac{As}{\partial} \left( 1 - \left( \frac{\tau}{s} \right)^{5/6} \right) \right]
\]

(39)

where \( \tau := \sqrt{\left( \text{dev} \sigma^p \right)^{\text{dev} \sigma^p}} \right] / 2 \) and \( \gamma_0, A = 39 \pi a^3 \mu \omega^2 / 16 \kappa \) are the material parameters. In (39), the athermal shear stress is taken to be different from \( s_0 \) in the original theory (Argon, 1973). In order to account for the pressure dependency of yielding as well as the succeeding true stress softening, we replace the original athermal shear strength \( s_0 \) with \( s := s + \gamma^p \) where \( s \) is a new material parameter controlling the pressure sensitivity of the yield stress. Its value ranges from 0.1 to 0.2 for most of glassy polymers, see e.g. Rabinowitz et al. (1970) and Bowden and Jukes (1972). The stress softening is incorporated by employing the phenomenological evolution rule for \( s \) proposed by Boyce et al. (1988)

\[
\ddot{s} = h(1 - s/s_0)^{\gamma^p} \quad \text{with} \quad s(0) = s_0,
\]

(40)

where \( h, s_0 \) are the additional material parameters describing the slope of the softening, initial and steady state values of the athermal shear strength \( s \), respectively.

Box 1: Algorithmic update of the plastic strains

1. Data Base. The history data \( \{ \varepsilon_0^p, s_0, \gamma_0^p, p_0 \} \) and the current total strain \( \varepsilon \) are given.
2. Explicit Update of the Athermal Shear Strength.
   \[
   \dot{s} = s_n + \Delta t (1 - s_n/s_0) \gamma_0^p + \varepsilon p_{\varepsilon}.
   \]
3. Implicit Update of the Plastic Strains.
   i) Set \( k = 0 \) and initialize \( \varepsilon^p|_{k=0} \leftarrow \varepsilon_0^p \)
   ii) Compute the dependent variables
       \[
       \gamma^p(39), \sigma(23), \beta(23), \sigma^p(24), \tau(39), \text{and } N(42)\]
   iii) Compute the residual and its norm
       \[
       r := \varepsilon^p - \varepsilon^p_0 - \Delta t \gamma^p \nabla, \quad ||r|| := \sqrt{r^T \cdot r}(45)
       \]
   iv) Compute the local tangent \( a := \partial a \cdot r \)
   v) Update plastic strains \( \varepsilon^p \leftarrow \varepsilon^p - a^{-1} \cdot r \)
   vi) Convergence check: If \( ||r|| \geq \text{tol}, k \leftarrow k + 1 \) goto ii) else continue with 4.
4. Store the history variables and proceed with the Consistent Moduli.
3.3. Algorithmic setting of the model

In the algorithmic treatment of the evolution equations, we consider an incremental formulation at discrete time steps \( \Delta t := t_{n+1} - t_n \) within a typical time interval \([t_n, t_{n+1}]\). All state variables at time \( t_n \) are given and in what follows indicated by the subscript \( n \).

3.3.1. Update of internal variables

The update of the plastic strain tensor \( \varepsilon^p \) and the athermal shear strength \( s \) is carried out by means of an algorithm that integrates the evolution equations (25) and (40) in the time interval. Here, we employ a fully explicit numerical integration scheme for the update of \( s \) through (40) and a fully implicit update scheme for \( \varepsilon^p \) via (25). The update of the athermal shear strength then gets the form

\[
\begin{align*}
    s &= s_n + \Delta t \tilde{s}_n = s_n + \Delta t h(1-s_n/s_{\infty})\tilde{\varepsilon}^p_n \quad \text{and} \quad \tilde{s} = s + s_p,
\end{align*}
\]

(41)

Owing to the explicit update of the athermal shear strength \( \tilde{s} \), hereafter it can be treated as a constant in the expressions containing \( \tilde{s} \). Use of the backward Euler update for \( \varepsilon^p \) leads us to the form

\[
\varepsilon^p = \varepsilon^p_n + \Delta t \dot{\varepsilon}^p N \quad \text{with} \quad N := \frac{\text{dev} (\varepsilon^p)}{||\text{dev} (\varepsilon^p)||}.
\]

This update equation of the plastic strains is non-linear due to implicit dependencies of \( \dot{\varepsilon}^p \) and \( N \) on the current value of \( \varepsilon^p \).

For this reason, a local Newton-type iterative update scheme has to be devised. The details of this conventional iterative method are outlined in Appendix. Basic steps of the algorithm are listed in Box 1 as well.

3.3.2. Algorithmic tangent moduli

In a typical implicit finite element analysis of a non-linear boundary value problem, global Newton-type iterative schemes necessitate the computation of the tangent moduli \( \mathbb{E}_{\text{algo}} \) being consistent with the numerical scheme used for the update of the internal variables. The consistent tangent moduli are defined as the sensitivity of the stress tensor to the conjugate logarithmic strain tensor

\[
\mathbb{E}_{\text{algo}} = \partial_{\varepsilon} \sigma = \mathbb{E}^e - 2\mu \hat{c} \varepsilon^p,
\]

where \( \mathbb{E}^e := \partial_{\varepsilon} \sigma = \kappa \mathbb{I} + 2\mu \hat{c} \) and \( \mathbb{I} \) is the symmetric fourth-order identity tensor.

Incorporation of the result (59) in (43) yields

\[
\mathbb{E}_{\text{algo}} = \mathbb{E}^e - 2\Delta t \mu \alpha^{-1} : \hat{\mathbb{I}} : \varepsilon^e.
\]

4. Illustrative numerical examples

This section is devoted to the assessment of the modeling capacity of the proposed approach by comparing its results to homogeneous as well as inhomogeneous experimental data. The homogeneous test data involve the true stress–true strain curves obtained from experiments conducted under different deformation rates and states on PMMA and PC. While the tensile stress–strain diagrams of the former are taken from the literature, Hope (1980), the compressive uniaxial and plane strain experiments on PC have been newly carried out. The results of both are then used for the identification of the adjustable material parameters. In addition to the homogeneous experiments on PC, a three-dimensional cold drawing of a dumbbell-shaped test piece, already depicted Fig. 1, was carried out. The data acquired from the inhomogeneous experiment contain not only the load–displacement diagram but also the three-dimensional surface strain fields. These results are compared with the finite element analysis of the cold drawing problem with the model parameters identified from the homogeneous experiments.

4.1. Investigations on homogeneous deformation states

As discussed in Section 1.1, the mechanical behavior of glassy polymers depends on many factors that involve loading rate, temperature, deformation state. In this section, we focus on the examples that particularly illustrate the rate and deformation state dependence of the stress–strain response of PMMA and PC, respectively.

The first set of experimental data, presented in Fig. 6a, was reported by Hope (1980). The data exhibit the rate-dependent tensile true stress–strain behavior of PMMA under different loading rates at \( \theta = 90 \ ^\circ \text{C} \). In order to investigate the rate-dependent behavior of PMMA, they employed waisted specimens with 5 mm waist width. These test pieces were then subjected to extension at different constant cross-head speeds. During the deformation, the lateral contraction of each specimen was recorded so that they were able to compute the true stress–strain curves for each constant cross-head speed but with varying true strain rate. Employing numerical differentiation and interpolation techniques on these data, they could extract the true stress–strain diagrams for the different true strain rates. Although it is a well known fact that the deformation of PMMA at
Fig. 6. Rate and deformation state dependencies in mechanical response of PMMA and PC. (a) True stress–true strain diagrams corresponding to the uniaxial tensile tests conducted at three different rates at \( \dot{\varepsilon} = 90 \, {^\circ} \) C. The set of material parameters used in the simulations are \( \kappa = 2633 \, {\text{MPa}}, \mu = 1003 \, {\text{MPa}}, \mu_s = 4.7 \, {\text{MPa}}, N_p = 3.5, \gamma_0 = 1.13 \times 10^{17} \, {\text{s}^{-1}}, A = 167 \, {\text{K/MPa}}, h = 250 \, {\text{MPa}}, s_0 = 90 \, {\text{MPa}}, s_a = 76 \, {\text{MPa}}, x = 0.2 \). (b) True stress–true strain diagrams of the uniaxial and the plane strain compression experiments carried out at true strain rate \( \ln \Lambda = 1 \times 10^{-5} \, {\text{s}^{-1}} \) at room temperature. The set of material parameters used in the simulations are \( \kappa = 2000 \, {\text{MPa}}, \mu = 900 \, {\text{MPa}}, \mu_s = 11.5 \, {\text{MPa}}, N_p = 2.35, \gamma_0 = 6.24 \times 10^{7} \, {\text{s}^{-1}}, A = 140 \, {\text{K/MPa}}, h = 500 \, {\text{MPa}}, s_0 = 102 \, {\text{MPa}}, s_a = 82 \, {\text{MPa}}, x = 0.11 \).

The uniaxial and plane strain compression experiments on polycarbonate (PC) samples depicted in Fig. 6b aim at presenting the deformation state dependence of the material response. The ductile PC is produced by Bayer AG in Leverkusen under a commercial name Makrolon 2607. Both experiments were conducted at a constant true strain rate \( \ln \Lambda = 1 \times 10^{-5} \, {\text{s}^{-1}} \) on a MTS servohydraulic uniaxial testing machine at room temperature. The rate of deformation was purposely selected to be slow enough to suppress the temperature increase due to dissipative heating. For the compressive uniaxial experiments, cylindrical PC specimens having a 8 mm diameter and a 8 mm height were employed. In the case of plane strain compression tests, however, cubic test pieces with an edge length of 8 mm were used. In both experiments particular attention has been paid to the appropriate lubrication between the contact surfaces of the specimen and the steel platens of the test machine in order to avoid the severe barreling appearing due to the friction developing under compression. For this purpose, a combination of Teflon film (solid lubricant) and commercial oil-based lubricant, WD-40, was employed as recently suggested in Dupaix and Boyce (2005). A drop of liquid lubricant was deposited between the lower metal plate and a Teflon film and also on the Teflon film itself. The PC sample was then placed on the film. The same procedure was repeated on the contact surface of the sample with the upper metal platen of the machine. This method eliminated the friction-induced barreling and allowed us to retain a macroscopically homogeneous shape of the test pieces throughout the tests.

Experimental results presented in Fig. 6b illustrate the typical yielding, stress softening and post-yield strain hardening behavior of glassy polymers under compression. As is commonly applied, the value of true stress was determined based on the incompressibility assumption. The deformation state dependence of the material response especially with regard to the yield stress and the post-yield strain hardening is in agreement with the observations reported in the literature, see for example Arruda and Boyce (1993a). The higher value of the yield stress encountered in the plane strain compression compared to the uniaxial compression is due to the excessive constraining boundary conditions in the plane strain deformation state and the pressure dependency of the yield stress, see Spitzig and Richmond (1979). In the case of plane strain compression chain molecules have a freedom to plastically align in only one direction. In the uniaxial compression, however, they can freely orient themselves symmetrically in the plane perpendicular to loading axis. If we consider those as nearly incompressible deformations, the chains aligning in a single direction in the plane strain compression state have to elongate more than...
the macromolecules stretch symmetrically in the uniaxial state. This leads to the apparent deformation state-dependent post-yield response and consequently evolution of anisotropy.

A further aim of the homogeneous tests on PC samples was the determination of the material parameters to be used in finite elements analysis of the cold drawing example on the same material partially presented in Sections 1.1 and 4.2. During the identification of the model parameters, we followed a way analogous to the one employed for the parameters of the data in Fig. 6a. The values of the model parameters given in the caption of Fig. 6 were first determined for the model based on the eight chain model kinematics, i.e. $m = 2$ for the micro-sphere model. The comparison of the simulations against the experimental results in Fig. 6b clearly shows that the proposed approach in the logarithmic strain space is able to capture the deformation state dependence of the yield stress and the post-yield hardening very well. Apart from the fittings based on the eight chain model (solid line), the effect of the non-affinity parameter $m$ of the micro-sphere model on the post-yield response is also investigated. The value of $m$ is varied from $m = 2$ to $m = 1.5, 2.5$. The larger the value of $m$, the stiffer the post-yield material behavior gets, see Fig. 6b. This provides an additional degree of freedom that serves to improve the post-yield fittings. Observe that the quality of the post-yield hardening simulation in the both uniaxial and plane strain cases has been slightly improved for the values of the non-affinity parameter $m$ greater than 2.

4.2. Cold drawing of a dumbbell-shaped PC specimen

In addition to the evaluation of the proposed approach with respect to the homogeneous experiments presented in the preceding section, we further test the capabilities of the proposed model with the parameters determined based on the homogeneous experiments against a three-dimensional cold drawing experiment. To this end, we consider a dumbbell-shaped PC test piece whose geometry is specified according to ISO 527 and also depicted in Fig. 7. The compressive uniaxial and plane strain stress–strain response of the material of interest is presented in Fig. 6b. The inhomogeneous tension experiment was carried out at a cross-head speed $\dot{u} = 2 \text{ mm/min}$ and analyzed with the optical measuring system called Aramis.

![Fig. 7. Geometry, boundary conditions and finite element discretization of the dumbbell-shaped polycarbonate test piece subjected to extension in the x-direction at the deformation rate $\dot{u} = 2 \text{ mm/min}$. All dimensions are given in millimeters.](image)

![Fig. 8. Simulation of the load–displacement curve of a dumbbell-shaped PC specimen subjected to extension at a cross-head speed $\dot{u} = 2 \text{ mm/min}$. The set of material parameters were determined based on the homogeneous uniaxial and plane strain compression experiments shown in Fig. 6b.](image)
The load–displacement diagram and the characteristics of the deformation process have been discussed in detail in Section 1.1. For the successful recognition of the three-dimensional surface of the specimen and its deformation via the grating method, the specimen must be coated in a specific manner depending on the kind of material to be tested. In the case of the transparent PC under the current investigation a suitable treatment for the surface is the dense-spraying of standard white glossy coating first, and next, while the former is still fresh, a more sparsely sprayed layer of matte graphite-based paint is superimposed. Once the specimen is prepared in this manner the test must be carried out immediately so that the paint does not fully dry and remains deformable throughout the experiment as depicted in Fig. 2. This will provide...
the contrast over the surface that the grating method requires for determining the deformation and hereby calculating the inhomogeneous three-dimensional strain field on the material. This is achieved by the use of a measuring arrangement with two CCD cameras. During the experiment the software acquires images with both cameras simultaneously allocating coordinates to every pixel on them. As a post-process the pixels of the recorded images are matched via mathematical transformations, see (Ritter, 1989). Once this has been done for the initial set of images, the process is repeated for the rest of the recorded stages of the deformation. From the difference of the coordinates of the pixels from the reference measurement to the others the displacement vectors are obtained. For further details on the grating method and the system Aramis, the reader is referred to Winter (1993), Bergmann and Ritter (1999) and ARAMIS User Manual (2001).

Fig. 10. Contour plots of the equivalent plastic strain $\|\varepsilon^p\|$ (left column) and the amount of plastic flow $\dot{\gamma}^p$ [s$^{-1}$] (right column) at the stages (a)-(h) as denoted in Fig. 1.
Apart from the dimensions of the dumbbell-shaped specimen, the boundary conditions and the finite element (FE) discretization of its geometry are depicted in Fig. 7. Owing to the apparent symmetries in its geometry, in the FE model of the specimen only its one quarter is discretized by 3750 eight-node Q1P0 mixed brick elements. While the end of the specimen at \( x = 0 \) mm is being fixed in all three directions, the degrees of freedom in \( y \)- and \( z \)-directions on its other end are restrained and the deformation in \( x \)-direction \( \dot{u}(t) \) is prescribed, see Fig. 7. Boundary conditions on the common facets with other quarters are governed by apparent geometrical symmetry conditions. The whole test piece is subjected to an extension at a cross-head speed \( \dot{u} = 2 \) mm/min at room temperature. In order to attain the neck initiating at the same place with the experiments, a slight geometrical imperfection at the end of the gauge section is imposed. The simulation of the global load–displacement response of the flat coupon extension is depicted in Fig. 8 in comparison with the experimental result. Characteristic features of the experimental load–displacement curve, which are discussed in detail in Section 1, are traced very well by the proposed model in the logarithmic strain space. Observe that the proposed model captures not only the load-level where the macro-yield occurs but also the amount of softening and the location of stress hardening where the neck reaches the end of the gauge section with the parameters determined from homogeneous compression experiments. This clearly justifies the procedure followed in identifying the model parameters and shows the multi-dimensional characteristics of the model.

In addition to the load–displacement diagram depicted in Fig. 8, the contour plots in Fig. 9 compare the field of thickness change during the cold drawing. The results obtained from the FE analysis (first and second columns) are compared with the measurements conducted by the optical measurement facility (third column). The labels of the rows (a)–(f) in Fig. 9 indicate the deformation stages corresponding to the levels labeled with the same letters as in Figs. 1 and 2. The field of thickness change up to the macro-yield, stages (a) and (b), is homogeneous throughout the test piece. The thickness change starts to localize in the softening branch between the load levels (b) and (d). It reaches the maximum value of 25% at stage (e) and is driven by the neck front along the gauge section. The computational results of the thickness change at almost all deformation stages quantitatively agree with the optical measurements. These quantitative results obtained from the simulation of the multi-axial inhomogeneous experiment once more indicate the validity of the proposed model.

The contour plots in Fig. 10 present the distributions of the equivalent plastic strain \( \|\varepsilon^p\| \) and the amount of plastic flow \( \dot{\varepsilon}^p \) on the left and the right columns, respectively. The labels of the rows (a)–(f) indicate the deformation stages corresponding to the levels labeled with the same letters as in Fig. 1. Although there is no geometrically apparent neck at the maximum load level (b), plastic flow starts to localize at the succeeding stage (c) at the location where the slight initial geometrical imperfection has been assigned. The stage (d) with the lowest post-yield load value corresponds to the stabilized state of the neck where the maximum plastic flow rate has been already achieved. At this stage the localized zone starts to separate at opposite directions drawing the shoulders of the neck towards the grips. The states (e),(f) and (g) illustrate the different degrees of the neck propagation where the progressive drawing of the material has been clearly exhibited. Owing to the unsymmetric initiation of the neck along the specimen, its propagation towards the right grip did not last as long as in the case of movement to the left end. When the neck shoulder reach the end of the gauge section, load deflection curve gets stiffer, stage (h).

The contour plots of the equivalent plastic strain field for the deformation stages (c)–(e) are repeated in Fig. 11 along with the macroscopic equivalent plastic strain contours at the depicted material points.

**Fig. 11.** Stereographic projection plots of the plastic stretch \( \varepsilon^p \) (33) corresponding to the three stages (c), (d) and (e) of the deformation are plotted along with the macroscopic equivalent plastic strain contours at the depicted material points.
5. Conclusion

We have developed a new constitutive model describing the finite viscoplastic deformation of ductile glassy polymers. The kinematical setting of finite viscoplasticity was laid out in the logarithmic strain space framed by purely geometric model-independent pre- and post-processing steps. This allowed us to construct the complete model within the framework akin to the geometrically linear theory. To our best knowledge, this is the first complete formulation of finite viscoplasticity of glassy polymers in the logarithmic strain space. For the modeling of the post-yield hardening both the eight chain model and the newly proposed non-affine micro-sphere models were considered and compared with respect to experimental data. The details of the three-dimensional implicit algorithm employed for the update of plastic strains were outlined in detail. In addition to the modeling and algorithmic aspects, new experimental data based on both homogeneous and inhomogeneous tests were reported. Besides the true stress-strain curves obtained from the homogeneous experiments on polycarbonate, the load–displacement diagram and the three-dimensional optical surface strain field measurements were presented. The proposed model was shown to be able to successfully capture various phenomena exhibited by glassy polymers. The constitutive model with the material parameters identified from homogeneous compression experiments was further compared with the results of the inhomogeneous tests. The results obtained indicate the outstanding performance of the proposed model and its high suitability for the FE analyses of boundary value problems.

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Appendix. Algorithmic setting of the constitutive model

A.1. Implicit update of plastic strains

In Section 3.3.1, we chose a fully implicit update scheme (42) for plastic strains $\varepsilon^p$. In order to start with the iterative scheme, we first introduce a non-linear residual function $r$ of the plastic strain tensor for a frozen deformation state $\varepsilon$ at time $t_{n+1}$:

$$
\mathbf{r}(\varepsilon^p) := \varepsilon^p - \varepsilon^n - \Delta t \varepsilon^p N = 0.
$$

The linearization of the residuum $\mathbf{r}$ is carried out at $k^{th}$ step of the Newton iteration about $\varepsilon^n_k$:

$$
\begin{align*}
\text{Lin} \mathbf{r}(\varepsilon^p)|_{\varepsilon^p_k} &= \mathbf{r}(\varepsilon^p_k) + \mathbf{a}_k : \Delta \varepsilon^p = 0,
\end{align*}
$$

where the local tangent of the Newton iteration is defined as

$$
a_k := \partial \mathbf{r}(\varepsilon^p_k) / \partial \varepsilon^p.
$$

The update equation for $\varepsilon^p$ at the $k^{th}$ step is then obtained by solving (46) for $\varepsilon^p$

$$
\varepsilon^p \leftarrow \varepsilon^p_k - a^{-1} \mathbf{r}(\varepsilon^p_k).
$$

The local tangent $a$ is computed by inserting the residual (45) into (47)

$$
a = \mathbb{I} - \Delta t \mathbf{h} : \partial_{\varepsilon^p} \text{dev}[\sigma^0],
$$

where we introduced the fourth-order tensor $\mathbb{h}$ defined by

$$
\mathbb{h} := \partial_{\text{dev}[\sigma^0]}(\varepsilon^p N) = (\alpha_1 \mathbb{I} + \alpha_2 N \otimes N)
$$

with the coefficients

$$
\alpha_1 := \frac{\varepsilon^p}{\| \text{dev}[\sigma^0] \|} \quad \text{and} \quad \alpha_2 := \alpha_1 \left( \frac{5}{6} \frac{A_s}{2 \overline{\sigma} (\frac{5}{2})^{5/6}} - 1 \right).
$$

For a frozen state of the total strain tensor $\varepsilon$, we have

$$
\partial_{\varepsilon^p} \text{dev}[\sigma^0] = \partial_{\varepsilon^p} \text{dev}[\sigma] - \partial_{\varepsilon^p} \text{dev}[\beta] = - (c^e + c^p),
$$

where $c^e := \partial_{\varepsilon^p} \text{dev}[\sigma]|_{\varepsilon^p} = - \partial_{\varepsilon^p} \text{dev}[\sigma]|_{\varepsilon} = 2\mu\varepsilon^p$ and $c^p := \partial_{\varepsilon^p} \text{dev}[\beta]$. Insertion of these results into (49) yields

$$
a = \mathbb{I} - \Delta t \mathbf{h} : (c^e + c^p).
$$

The explicit form of $c^p$ directly depends on the network model employed for modeling the back stresses $\beta$. For the sake of brevity, we here consider $c^p$ corresponding only to the eight chain model. To this end, we retrieve the definition of back stresses in (35) and recast it into the spectral form of a tensor-valued isotropic function of the plastic strains.
\[ \text{dev} \beta_3 = \frac{1}{2} \sum_{A=1}^{3} \beta_A \mathbf{n}_A^p \otimes \mathbf{n}_A^p, \]

where \( \beta_A = \beta_A - \frac{1}{2} \sum_{B=1}^{3} \beta_B \) denote the eigenvalues of the deviatoric back stress tensor with \( \beta_A = \rho_c (\sigma_{ec}^p \exp(2\epsilon_{ec}^p)) \) and \( \mathbf{n}_A^p \) stand for its eigenvectors. Having introduced the spectral form of \( \text{dev} \beta_3 \), its derivative with respect to \( \epsilon^p \) can be obtained by

\[ c^p := \partial_{\epsilon^p} (\text{dev} \beta_3) = \sum_{A=1}^{3} \sum_{B=1}^{3} c_{AB} \mathbf{m}_A^p \otimes \mathbf{m}_B^p + \sum_{A=1}^{3} 2 \frac{\beta_A - \beta_B}{\epsilon_A^p - \epsilon_B^p} (\xi_{AB} + \xi_{BA}), \]

where \( \mathbf{m}_A^p := \mathbf{n}_A^p \otimes \mathbf{n}_A^p \), \( \xi_{AB} = \frac{m_{AB}}{C_{10}} \) and \( \mathbf{m}_A^p \) stand for the derivatives of the principal backstresses \( \beta_A \) with respect to the plastic eigengra\v{s}tress \( \epsilon^p_A \). Their explicit form is readily determined from the definition of the principal backstresses \( \beta_A \)

\[ c_{KL} := \partial_{\epsilon^p} \beta_K = \frac{\rho_c (\epsilon_{ec}^p)}{3 \epsilon_{ec}^p} \exp(2\epsilon_{ec}^p) \exp(2\epsilon_{ec}^p) + 2 \rho_c (\epsilon_{ec}^p) \exp(2\epsilon_{ec}^p) \delta_{KL}, \]

where \( \rho_c (\epsilon_{ec}^p) := \partial_{\epsilon^p} \rho_c = 4 \mu_c (\epsilon_{ec}^p - N_p)/(3(N_p - \epsilon_{ec}^p)^2) \) and \( \delta_{KL} \) denotes the Kronecker delta. Observe that the spectral form of \( c^p \) does not incorporate the cases where the equal eigenvalues lead to singularities in the second term of (54). For the treatment of these cases by limits and further details concerning representations in the eigen-space, the reader is referred to Ogden (1984), Šilhavy (1997), Miehe and Lambrecht (2001) among others.

A.2. Sensitivity of \( \epsilon^p \) with respect to \( \epsilon \)

Use of a stable implicit scheme for the update of internal variables allows one to use larger time steps. Computation of the consistent tangent moduli, however, requires the sensitivity of strain-like internal variables to a total strain measure. For the present case, the sensitivity of \( \epsilon^p \) to \( \epsilon \) can be computed from the persistency condition implying the steady fulfillment of vanishing residuum defined in (45). Therefore, the total derivative of the residuum must also be zero at any instant of the deformation, i.e.

\[ d_\epsilon r = \partial_{\epsilon^p} r^p + \partial_{\epsilon^p} r^p : \partial_{\epsilon^p} \epsilon^p = 0. \]

The left contractor of the second term is the local tangent \( \partial_{\epsilon^p} r^p \) that has been already computed in the last local Newton iteration step in (52). The desired derivative can then be obtained from the condition (56) as

\[ \partial_{\epsilon^p} \epsilon^p = -a^{-1} : \partial_{\epsilon^p} r^p. \]

Recalling the definition of the residuum in (45), the derivative \( \partial_{\epsilon^p} r^p \) can be expressed in a form analogous to (49)

\[ \partial_{\epsilon^p} r^p = -\Delta t h : c^p, \]

where the tensor \( h \) has been already defined in (50). Finally, the insertion of (58) into (57) leads us to the desired sensitivity

\[ \partial_{\epsilon^p} \epsilon^p = \Delta t a^{-1} : h : c^p. \]

References


