Mechanics of Materials 80 (2015) 37–51

Contents lists available at ScienceDirect

Mechanics of Materials

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

# Statistical-mechanics based modeling of anisotropic viscoplastic deformation

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ARTICLE INFO

*Article history:*
Received 1 November 2013
Received in revised form 25 September 2014
Available online 6 October 2014

*Keywords:*
Anisotropic material (B)
Constitutive behavior (B)
Elastic–viscoplastic material (B)
Nonequilibrium statistical mechanics

ABSTRACT

Statistical mechanics-based coarse graining is used for constitutive modeling of finite elasto-viscoplastic deformation behavior of transversely isotropic materials, without relying on the associated flow rule or classical yield criteria. It was shown previously (Hütter and Tervoort, 2008c) that a detailed expression for the plastic velocity gradient can be obtained in terms of correlations of the fluctuations of the elastic deformation gradient. In this paper, we demonstrate that it is crucial to include cross-correlations between fluctuations of different components of the elastic deformation gradient in order to describe materials with strong plastic anisotropy. Subsequently, the expression for the equivalent stress is obtained from a steady-state analysis during plastic deformation, and is shown to coincide with the Hill equivalent stress in the limit of small elastic deformations. In this case, only two material parameters describe in a self-consistent manner the anisotropic structure of both the plastic velocity gradient and the equivalent stress. Finally, the new constitutive viscoplastic description is successfully applied to describe experimental yield data of oriented isotactic polypropylene, specifically the influence of anisotropy and deformation rate on yielding. Particularly, a step-by-step procedure is given to identify all model parameters.



## 1. Introduction

Solid state processing of polymers and metals involving large plastic deformations, such as rolling, forging and drawing, often results in materials exhibiting profound anisotropic deformation behavior, that needs to be considered during subsequent applications of the material in use. In case of polymeric materials, the plastic flow behavior can also be strongly rate- and temperature-dependent, adding additional complexity to the mechanical behavior. Most challenging in this respect, and, therefore, still a topic of active research, is to find a concise description of the finite three-dimensional anisotropic elasto-viscoplastic behavior of these materials, by selecting the most relevant internal variables, complemented with a minimum amount of material constants, combined with a detailed procedure for the experimental determination of these material constants.

Hill was the first to consider rate-independent anisotropic yielding at small deformations, by extending the quadratic yield criterion of Von Mises for isotropic materials to orthorhombic and transversely isotropic materials (Hill, 1948, 1950). The Hill criterion is still very much applied today and has been used extensively as a starting point for elasto-viscoplastic modeling of finite anisotropic yield behavior. For this, typically, the invariant formulation of the Hill criterion is used as a plastic potential to obtain the direction of plastic flow, assuming the associated flow rule (Hill, 1950) to hold for anisotropic materials. The equivalent plastic strain rate is then obtained from the

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http://dx.doi.org/10.1016/j.mechmat.2014.09.007
0167-6636/

consistency condition, or defined as being work conjugate to the Hill equivalent stress (Dafalias, 2000; Hill, 1987; Pereda et al., 1993; Van Erp et al., 2009). In addition, constitutive equations must be provided for the so-called plastic spin, to describe the deviation of the spin of the material axes from the continuum spin (Loret, 1983; Dafalias, 1985; Loret and Dafalias, 1992; Dafalias, 1998).

To find a constitutive relation for the plastic strain-rate tensor (plastic velocity gradient) from first principles, relating the kinetics of plastic flow to the state of the material, without help of the associated flow rule, is non-trivial, especially for anisotropic materials. Thermodynamics can be employed as a guardrail. For example, continuum thermodynamics (Šilhavý, 1997) and the general equation for the non-equilibrium reversible–irreversible coupling (GENERIC) (Grmela and Öttinger, 1997; Öttinger and Grmela, 1997; Öttinger, 2005) can be employed, and a recent discussion has shown that these methods lead to comparable constraints on the plastic velocity gradient (Hütter and Svendsen, 2012). However, the tensorial structure of the plastic velocity gradient cannot be reduced sufficiently by such thermodynamic constraints alone, and, hence, other methods must be employed to avoid arbitrary ad hoc assumptions. Possible tools for studying the tensorial structure are the tensorial representation theorems, that however typically result in an unrealistically large number of material constants (Loret, 1983; Hütter and Tervoort, 2008b).

Statistical mechanics at equilibrium is a tool, allowing one to calculate (static) macroscopic equilibrium properties based on the laws that govern the dynamics of the microscopic constituents (e.g. Lifshitz and Pitaevskii (1980)). Similarly, procedures have emerged to access transport coefficients, e.g., thermal conductivity and viscosity, based on the microscopic dynamics in the form of so-called fluctuation–dissipation relations (e.g. Kubo et al. (1991)). Such procedures can be abstracted, using the projection-operator method (Grabert, 1982), within the nonequilibrium thermodynamics framework GENERIC (Öttinger, 1998, 2005). We have recently shown that dynamic coarse-graining in the form of fluctuation–dissipation relations can be employed to aid constitutive modeling of the plastic velocity gradient (Hütter and Tervoort, 2008c).

It is the objective of this paper to further exploit thermodynamically-guided dynamic coarse-graining, by deriving a constitutive law for the plastic velocity gradient from a generalized fluctuation–dissipation relation, thereby modeling anisotropic elasto-viscoplasticity without relying on classical yield criteria or the associated flow rule. We shall restrict our attention to transversely isotropic materials.

The manuscript is organized as follows: Section 2 briefly recapitulates the main results of earlier efforts (Hütter and Tervoort, 2008c) to relate the viscoplastic material behavior to fluctuations in the elastic deformation. Based thereon, the main achievements of this paper are presented, namely the importance of fluctuation cross-correlations, the specification of the constitutive rule for the plastic velocity gradient, and the definition of a scalar measure of stress, the so-called equivalent stress. In Section 3, it is demonstrated in detail how to use the resulting model for describing experimental yield stress data of an oriented solid polymer depicting rate-dependent transverse isotropic yield behavior. Particularly, the proper procedure for identifying the model parameters is discussed in detail. Section 4 concludes the manuscript with a discussion.

## 2. Plastic deformation of transversely isotropic materials

### 2.1. Starting point and notation

This section gives a concise summary of results from our previous publications (Hütter and Tervoort, 2008a,b,c). Thereby, the notation and background are introduced that are used for the development of the new achievements of this paper, starting with Section 2.2.

An important first step when using coarse graining towards macroscopic dynamic properties is to specify those quantities of which the fine-scale fluctuations give rise to the macroscopic dynamic behavior. In previous work, we have identified the elastic deformation gradient $\boldsymbol{F}^{\mathrm{e}}$ as a convenient internal variable to model thermoelasticity and elasto-viscoplasticity of anisotropic solids (Hütter and Tervoort, 2008a,b). Note that in this setting, the choice of $\boldsymbol{F}^{\mathrm{e}}$ as internal variable does not rely on a multiplicative decomposition of the total deformation gradient $\boldsymbol{F}$, nor on kinematic assumptions regarding intermediate configurations. In case of pure elastic (affine) deformations, the elastic deformation gradient $\boldsymbol{F}^{\mathrm{e}}$ coincides with the total deformation gradient $\boldsymbol{F}$, while the onset of irreversible viscoplastic (and hence non-affine) deformation impedes further growth of the elastic deformation. This suggests the following evolution equation for $\boldsymbol{F}^{\mathrm{e}}$ to describe the accumulation of elastic strain, retarded by a plastic strain rate (Hütter and Tervoort, 2008b; Besseling and van der Giessen, 1994, Chapter 7),

$$D_t\boldsymbol{F}^{\mathrm{e}} = \boldsymbol{L}\cdot\boldsymbol{F}^{\mathrm{e}} - \boldsymbol{L}^{p,c}\cdot\boldsymbol{F}^{\mathrm{e}} \tag{1a}$$

$$= \boldsymbol{L}\cdot\boldsymbol{F}^{\mathrm{e}} - \boldsymbol{F}^{\mathrm{e}}\cdot\boldsymbol{L}^{p,r}, \tag{1b}$$

which reduces in the linear regime to the well-known additive decomposition of the total strain rate tensor into its elastic and viscoplastic contributions (Besseling and van der Giessen, 1994, Chapters 1 and 4). In Eq. (1), we adopt an Eulerian formulation with $D_t = \partial_t + \boldsymbol{v}\cdot\nabla$ denoting the material derivative. The first term on the right-hand side (r.h.s.) describes the affine part of the deformation using the total velocity gradient, $\boldsymbol{L} = (\nabla\boldsymbol{v})^T$. The difference between the elastic and total deformation gradient originates from the second term on the r.h.s., representing the rate of plastic deformation. The latter can be captured in two equivalent forms, namely by the plastic velocity gradient tensor in the current and reference configuration, $\boldsymbol{L}^{p,c}$ and $\boldsymbol{L}^{p,r}$, respectively.

We have shown in our earlier work (Hütter and Tervoort, 2008c) that, in a closed nonisothermal model, the specification of the plastic velocity gradient follows from fluctuations $\dot{\boldsymbol{F}}^{\mathrm{e,f}}$ of the elastic deformation gradient $\boldsymbol{F}^{\mathrm{e}}$. The fluctuations $\dot{\boldsymbol{F}}^{\mathrm{e,f}}$ originate from the dynamics of the underlying molecular structure. For illustration purposes, these fluctuations are, on the coarse scale, assumed to obey white-noise statistics, i.e. memory-less