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A Geometrically Nonlinear Elasto-Viscoplasticity Theory of Second Grade

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A general concept for the consideration of the influence of strain gradients on elasto-viscoplastic material behaviour at finite deformation is presented that does not need to account for an additional flow rule for the plastic strain gradient. The balance of momentum including the representation of the stresses, the power of work at contact for the formulation of boundary conditions as well as the nonlocal form of the total power of deformation are derived via the dissipation inequality for the investigated nonpolar continuum model of second grade. In addition to the gradient of the elastic strain tensor, energy storage with gradients of different internal variables is considered: gradient of (i) the plastic strain tensor itself, (ii) an internal strain tensor induced by viscoplastic straining, by which energy due to hardening is stored also with its gradient, and (iii) scalar internal variables like the accumulated viscoplastic strain or an internal time variable of damage. Finally, for the simulation of the damage behaviour during a strain hold-time period at a crack tip the responses of a rate-dependent and a quasi-rate-independent gradient-enhanced damage model are compared in finite element studies.

1 Introduction

When a significant gradient of macroscopic loading is already present across the size of the relevant substructure (e.g. dislocation arrangements, polymer chains, particles, grains, voids, cells of a foam) then the macroscopic strain or an internal variable can not be considered as constant anymore within a macroscopic continuum element which has to cover the heterogeneity of the material. Thus, the influence of that spatial gradient of loading on the material behaviour within a macroscopic continuum element should be taken into account (see, e.g., Aifantis, 1987; Fleck et al., 1994; Gao et al., 1999; Hutchinson, 2000). For example, although the problem of localization is mathematically well-posed for a rate-dependent pure local constitutive model (Needleman, 1988), a narrow localization zone can be influenced by the structure of the material, and this gives rise to the introduction of a substructure-related intrinsic length-scale. The viscosity of the model must describe primarily the physical rate-dependence of the material at homogeneous deformation and is then already fixed by that.

Examples for locations of strong spatial gradients of the macroscopic strain field are: the interfaces (e.g. Busso et al., 2000; Borg et al., 2006; Cordero et al., 2010), the grain boundary of a bicrystal (Shu & Fleck, 1999; Cermelli & Gurtin, 2002) or within a polycrystal (e.g. Smyshlyaev & Fleck, 1996; Evers et al., 2004; Cheong et al., 2005), the interface of a thin film (e.g. Fredriksson & Gudmundson, 2005), the zone under an indenter (e.g. Nix & Gao, 1998; Shu & Fleck, 1998; Wei & Hutchinson, 2003), the strain field at a reinforcement in a metal matrix composite (Zhu et al., 1997; Shu & Barlow, 2000; Niordson, 2003), the constrained deformation of a cellular material (Chen et al., 1998; Chen & Fleck, 2002), a shear band (e.g. Aifantis, 1984; Coleman & Hodgdon, 1985; Zbib & Aifantis, 1988; Mühlhaus & Aifantis, 1991a; Zhu et al., 1995; Forest, 1998a; Shi et al., 2000; Batra & Chen, 2001; Reusch et al., 2003a,b; Forest & Lorentz, 2004) or a crack tip (e.g. Xia & Hutchinson, 1996; Feucht, 1998; Forest et al., 2001; Hwang et al., 2003; Reusch, 2003; Wei et al., 2004; Levkovitch et al., 2005).

Not only strain gradient plasticity effects in metals have been investigated, but also size-effects in polymers were considered at pure elastic torsion and bending (Aifantis, 1999a; Lam et al., 2003), at fibre pull-out (Tenek & Aifantis, 2001) and at indentation (Lam & Chong, 1999; Chong & Lam, 1999). Another example for a strong gradient of macroscopic loading on a heterogeneous material can be the constrained deformation of a polymeric foam (Aifantis, 1999a, and the literature cited therein).

Generalized, i.e. Cosserat or micromorphic, continua (e.g., Germain, 1973b; Eringen, 1999; Forest & Sievert, 2003, 2006) are well-suited for the description of inhomogeneous deformation behaviour with an internal degree

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of freedom, i.e. when a substructure-deformation independently from the macroscopic displacement field is present. Such a pronounced substructure can be, for example, the reinforcement of a composite (like fibres, Besdo & Dorau, 1988; Fleck & Shu, 1995; Forest, 1998b; or like layers of a laminate, e.g. Mühlhaus, 1995), granular materials (like rock-structures, e.g., Besdo, 1985; Mühlhaus, 1989; or like soil, e.g. Ehlers & Volk, 1998) or the cellular structure of a foam (Forest et al., 2005; Dillard et al., 2006). The micropolar modelling is also applicable to the description of lattice defects in crystals (Forest, et al., 1997; Clayton et al., 2006). The consideration of the lattice rotation (rotational part of the finite elastic deformation) and its gradient (e.g. Le & Stumpf, 1996; Shizawa & Zbib, 1999; Acharya & Bassani, 2000) is also in the direction towards a micropolar theory. However, if an independent deformation of the substructure is not significant, but a strong gradient of the macroscopic loading is present across the size of the relevant substructure nevertheless, then a model extended by spatial gradients of stain-like internal variables or higher gradients of the symmetric displacement-strain seems to be appropriate. This will be considered in the present work for the first gradients of finite elasto-viscoplastic deformations.

First strain gradient models were developed by Toupin (1962), Koiter (1964) and Mindlin (1964) in elasticity theory. Germain (1973a) formulated the principle of virtual power for a second gradient theory in the current placement. Leroy & Molinari (1993) have extended the elasticity theory of Mindlin (1965) to finite deformation using the gradient with respect to the reference placement. Eringen (1966), Dunn & Serrin (1985) and Trostel (1985) developed higher gradient theories also with respect to dissipative behaviour. Early approaches to elastoplastic strain gradient theories go back to Green et al. (1968), Dillon & Kratochvil (1970) and Wright & Batra (1987). Besides an elastic strain gradient they also considered a plastic strain gradient, i.e. written for small deformations, $\text{grad}\,\boldsymbol{\varepsilon} = (\text{grad}\,\boldsymbol{\varepsilon})_e + (\text{grad}\,\boldsymbol{\varepsilon})_p$, and introduced an independent flow rule for the third-order tensor $(\text{grad}\,\boldsymbol{\varepsilon})_p$. These strain gradient parts are generally different from the gradients of the elastic and plastic strain, i.e., $\text{grad}\,\boldsymbol{\varepsilon} = \text{grad}\,\boldsymbol{\varepsilon}_e + \text{grad}\,\boldsymbol{\varepsilon}_p$ (for small deformations). For example, at zero spatial gradient of elastic strain, $\text{grad}\,\boldsymbol{\varepsilon}_e = \mathbf{0}$, an elastic strain gradient is generally still present and equal to the deviation of the plastic strain gradient from the gradient of plastic strain: $(\text{grad}\,\boldsymbol{\varepsilon})_e = \text{grad}\,\boldsymbol{\varepsilon}_p - (\text{grad}\,\boldsymbol{\varepsilon})_p$. This type of theory was followed, e.g., by Fleck & Hutchinson (1993, 1997) and Chambon et al. (2004).

In the last decades several models have also been developed taking into account the influence of the gradient of the plastic strain or of an internal variable (e.g., Aifantis, 1984, 1999b, 2003; Maugin, 1990; Mühlhaus & Aifantis, 1991b; Vardoulakis & Frantziskonis, 1992; Nagdhi & Srinivasa, 1993; Valanis, 1996; Frémond & Nedjar, 1996; Steinmann, 1996; Sievert et al., 1998; Svendsen, 1999, 2002; Menzel & Steinmann, 2000; Gurtin, 2000, 2004; Fleck & Hutchinson, 2001; Huang et al., 2001; Forest et al., 2002; Gudmundson, 2004; Geers, 2004; Gurtin & Anand, 2005b, 2009; Polizzotto, 2009). Polizzotto (2003) investigated the first and the second spatial gradient of either the accumulated plastic strain or of the strain in elasticity for small deformations. Forest & Sievert (2003) and Polizzotto (2007) also developed a model which takes into account the gradient of the plastic strain tensor as well as of the elastic strain part for the geometrically linear case.

Analogously to the balance equation of the fundamental strain gradient theory of Mindlin (1965) evolution equations for the viscoplastic strains will be derived in the present work directly from the basic constitutive property of energy storage with the first gradients of elastic as well as plastic strains at finite deformation via the general dissipation inequality. The resulting evolution equations have the same tensor-order as for simple material behaviour but include spatial derivatives and that of even order.

For a thermomechanical derivation of the theory we start from the basic principles of thermodynamics. The energy balance reads as

$$\rho\,\dot{e} + \tfrac{1}{2}\rho\,(\dot{\mathbf{u}}^2)^{\cdot} = \rho\,p_b + \mathbf{w}\cdot\boldsymbol{\nabla} - \mathbf{q}\cdot\boldsymbol{\nabla} \tag{1.1}$$

with the internal energy e, the heat flux vector $\mathbf{q}$, the work flux vector $\mathbf{w}$ (cf. Dunn & Serrin, 1985), i.e. the vector of the power of work at contact, with the power p_b of body forces (neglecting the external heat supply), the nabla operator $\boldsymbol{\nabla}$ and the mass density ρ in the initial placement of the body and with the displacement vector $\mathbf{u}$ with respect to this reference placement.

The inequality for the local entropy η is

$$\rho\,\dot{\eta} + \mathbf{j}\cdot\boldsymbol{\nabla} \geq 0 \qquad , \qquad \mathbf{j} \equiv \mathbf{q}/\theta \tag{1.2}$$

where $\mathbf{j}$ denotes the entropy flux and θ the temperature. No extra entropy flux is assumed here for the description of solids, although this could be considered for internal variables influencing the heat conduction inequality (Maugin, 1990).

The required additional boundary conditions for the evolution equations in terms of partial differential equations are given in the present gradient theory by an higher-order power of surface work, i.e. an extra energy flux included in the work flux $\mathbf{w}\cdot\mathbf{n}$ on the surface of a body ($\mathbf{n}$ being the outward unit normal to the surface in the initial placement).

Introducing the Helmholtz free energy $\psi := e - \eta\,\theta$, the Clausius-Duhem inequality results from combining the entropy inequality (1.2) with the energy balance (1.1) in the form

$$\rho\, p_b - \tfrac{1}{2}\rho\,(\dot{\mathbf{u}}^2)^{\dot{}} + \mathbf{w}\cdot\nabla \;-\; \rho(\dot{\psi} + \eta\,\dot{\theta}) - \mathbf{q}/\theta\cdot\nabla\theta \;\geq\; 0 \qquad (1.3)$$

With respect to the temperature gradient this can be identically fulfilled by the classical Fourier's law $\mathbf{q} = -\boldsymbol{\kappa}\cdot\nabla\theta$, and the inequality of the mechanical dissipation power d then remains

$$\rho\, d := \rho\, p_b - \tfrac{1}{2}\rho\,(\dot{\mathbf{u}}^2)^{\dot{}} + \mathbf{w}\cdot\nabla \;-\; \rho(\dot{\psi} + \eta\,\dot{\theta}) \;\geq\; 0 \qquad (1.4)$$

The local deformation $\mathbf{F}$ is defined with respect to the initial placement of the considered process

$$\mathbf{F} \;=\; \mathbf{1} + \mathbf{u}\otimes\nabla \qquad (1.5)$$

For the tensor notation used see appendix A.

2 Strain Energy Storage and Dissipation

2.1 Elastic-plastic decomposition of the local deformation

The considered materials can deform also without mechanical dissipation power in the current configuration, i.e. having an elastic part of deformation. Thus, the remainder of the total strain can evolve only together with mechanical dissipation power, called plastic deformation. In this work, the word "plastic" deformation stands generally for an "inelastic", i.e. dissipative, deformation which can be rate-dependent. The elastic-plastic decomposition of the local deformation according to Mandel (1971) and Rice (1971) is adopted

$$\mathbf{F} \;=\; \tilde{\mathbf{R}}\,\mathbf{U}_e\,\mathbf{F}_p \qquad (2.1)$$

with a proper orthogonal tensor $\tilde{\mathbf{R}}$ describing the rigid rotation of the strained material element. If one assumes, for pure local constitutive modelling, that the elastic constitutive law for the stress tensor related to the current configuration has, even after large plastic deformations, the same form as in the pure hyperelastic case, then the elastic-plastic decomposition of deformation (2.1) is not only sufficient but also necessary for that form of the hyperelastic stress-strain law (Sievert, 1993; for the proof see Sievert, 1997, or in Besson et al., 2001, pp. 311). The decomposition (2.1) of the total deformation into an elastic and an inelastic part is also used in viscoelasticity modelling (see, e.g., Sidoroff, 1974; Krawietz, 1986; Lion, 1997; Reese & Govindjee, 1998; Drozdov et al., 2003; Ehlers & Markert, 2003).

For anisotropic materials the generally non-symmetric tensor $\mathbf{F}_p$ describes the plastic deformation of a material element with respect to material (anisotropy) directions (Mandel, 1974; Rice, 1975) and is thus invariant under observer transformation (compare Gurtin, 2000). Material directions can be already initially present (as crystal axes or fibre directions) as well as plastically induced (texture axes). If the material directions are deforming elastically like the line elements of the macroscopic continuum element (in contrast to a micropolar continuum), then they are stretched simply with $\mathbf{U}_e$, too. In this case $\tilde{\mathbf{R}}$ also represents the mean rotation of the material directions, e.g. the lattice rotation, with respect to the observer-frame.

Under an Euclidean observer transformation with a proper orthogonal tensor $\mathbf{Q}(t) =: \mathbf{Q}_t$, indicated by stars on the transformed measures, the local deformation is transformed as

$$\mathbf{F}^* = \tilde{\mathbf{R}}^* \, \mathbf{U}_e^* \, \mathbf{F}_p^* = \mathbf{Q}_t \, \mathbf{F} = \mathbf{Q}_t \, \tilde{\mathbf{R}} \, \mathbf{U}_e \, \mathbf{F}_p \tag{2.2}$$

Thus, as $\mathbf{F}_p$, also $\mathbf{U}_e$ and therewith the elastic Cauchy-Green tensor $\mathbf{C}_e := \mathbf{U}_e^2$ are invariant under change of observer for $\tilde{\mathbf{R}}^* = \mathbf{Q}_t \, \tilde{\mathbf{R}}$.

At symmetry transformation by pre-rotation of the material element with $\mathbf{Q}_0$, indicated by a superscript $^+$,

$$\mathbf{F}^+ = \tilde{\mathbf{R}}^+ \, \mathbf{U}_e^+ \, \mathbf{F}_p^+ = \mathbf{F} \, \mathbf{Q}_0 = \tilde{\mathbf{R}} \, \mathbf{U}_e \, \mathbf{F}_p \, \mathbf{Q}_0 \equiv \tilde{\mathbf{R}} \, \mathbf{Q}_0 \, \mathbf{Q}_0^{\mathrm{T}} \, \mathbf{U}_e \, \mathbf{Q}_0 \, \mathbf{Q}_0^{\mathrm{T}} \, \mathbf{F}_p \, \mathbf{Q}_0 \tag{2.3a}$$

$\mathbf{U}_e$ and $\mathbf{F}_p$ are back-rotated with respect to the material

$$\mathbf{U}_e^+ = \mathbf{Q}_0^{\mathrm{T}} \, \mathbf{U}_e \, \mathbf{Q}_0 \quad , \quad \mathbf{F}_p^+ = \mathbf{Q}_0^{\mathrm{T}} \, \mathbf{F}_p \, \mathbf{Q}_0 \quad , \quad \tilde{\mathbf{R}}^+ = \tilde{\mathbf{R}} \, \mathbf{Q}_0 \quad . \tag{2.3b}$$

The deformation rate of the current configuration is

$$\dot{\mathbf{F}} \, \mathbf{F}^{-1} = \dot{\tilde{\mathbf{R}}} \, \tilde{\mathbf{R}}^{\mathrm{T}} + \tilde{\mathbf{R}} \, \dot{\mathbf{U}}_e \mathbf{U}_e^{-1} \, \tilde{\mathbf{R}}^{\mathrm{T}} + \tilde{\mathbf{R}} \, \mathbf{U}_e \, \dot{\mathbf{F}}_p \mathbf{F}_p^{-1} \, \mathbf{U}_e^{-1} \, \tilde{\mathbf{R}}^{\mathrm{T}} \tag{2.4}$$

Thus, the elastic strain-rate of the current configuration can be represented as

$$\left(\dot{\mathbf{U}}_e \mathbf{U}_e^{-1}\right)_{\mathrm{s}} = \tilde{\mathbf{R}}^{\mathrm{T}} \left(\dot{\mathbf{F}} \, \mathbf{F}^{-1}\right)_{\mathrm{s}} \tilde{\mathbf{R}} - \left(\mathbf{U}_e \, \dot{\mathbf{F}}_p \mathbf{F}_p^{-1} \, \mathbf{U}_e^{-1}\right)_{\mathrm{s}} \tag{2.5}$$

The rate of the elastic Cauchy-Green tensor $\mathbf{C}_e := \mathbf{U}_e^2$ is

$$\dot{\overline{\left(\mathbf{U}_e^2\right)}} = \mathbf{U}_e \dot{\mathbf{U}}_e + \dot{\mathbf{U}}_e \mathbf{U}_e = \mathbf{U}_e (\dot{\mathbf{U}}_e \mathbf{U}_e^{-1} + \mathbf{U}_e^{-1} \, \dot{\mathbf{U}}_e) \, \mathbf{U}_e = \mathbf{U}_e \, 2 (\dot{\mathbf{U}}_e \mathbf{U}_e^{-1})_{\mathrm{s}} \, \mathbf{U}_e \tag{2.6}$$

2.2 Evaluation of the dissipation inequality

At energy storage with the gradient of elastic strain one has generally to consider a gradient of thermal strain, too, i.e., a stress-free strain gradient due to a temperature gradient (Cardona et al., 1999). First steps towards a consideration of the temperature gradient also in the free energy were undertaken by Eringen (1966), Batra (1975), Forest et al. (2000), Ireman & Nguyen (2004), Nguyen & Andrieux (2005) and Forest & Amestoy (2008). But for clarity of the presentation of the geometrically nonlinear gradient elasto-viscoplasticity theory including, e.g., kinematic hardening, this work will be restricted to isothermal or locally isocaloric (and thus isentropic: $\rho d - \mathbf{q} \cdot \nabla = \theta \dot{\eta}$) processes. Therefore, the mechanical dissipation power d will be called in the following in short dissipation power.

Strain energy storage also with gradients of the elastic strain as well as of observer-invariant internal variables $\boldsymbol{\alpha}$ is represented by

$$\rho \psi = \hat{\psi}\left(\mathbf{C}_e , \mathbf{C}_e \otimes \nabla, \boldsymbol{\alpha}, \boldsymbol{\alpha} \otimes \nabla\right) \tag{2.7}$$

By time derivation of the strain energy function (2.7) one gets, using the material time derivative and spatially partial integration:

$$\begin{aligned} \rho \dot{\psi} = & \left(\dot{\mathbf{C}}_e \cdot\cdot \frac{\partial \hat{\psi}}{\partial \mathbf{C}_e \otimes \nabla}\right) \cdot \nabla + \dot{\mathbf{C}}_e \cdot\cdot \left(\frac{\partial \hat{\psi}}{\partial \mathbf{C}_e} - \frac{\partial \hat{\psi}}{\partial \mathbf{C}_e \otimes \nabla} \cdot \nabla\right) \\ & + \left(\dot{\boldsymbol{\alpha}} \cdot \frac{\partial \hat{\psi}}{\partial \boldsymbol{\alpha} \otimes \nabla}\right) \cdot \nabla + \dot{\boldsymbol{\alpha}} \cdot \left(\frac{\partial \hat{\psi}}{\partial \boldsymbol{\alpha}} - \frac{\partial \hat{\psi}}{\partial \boldsymbol{\alpha} \otimes \nabla} \cdot \nabla\right) \end{aligned} \tag{2.8}$$

Using eq. (2.6) the rate of strain energy storage can be expressed as

$$\rho\dot{\psi} = \left((\dot{\mathbf{U}}_e \mathbf{U}_e^{-1})_s \cdot\cdot\, \mathbf{T}^R \right) \cdot \nabla + (\dot{\mathbf{U}}_e \mathbf{U}_e^{-1})_s \cdot\cdot\, \boldsymbol{\tau}^R + (\dot{\boldsymbol{\alpha}} \cdot \mathbf{B}) \cdot \nabla + \dot{\boldsymbol{\alpha}} \cdot \mathbf{a} \tag{2.9}$$

with the observer-invariant Kirchhoff stress tensors

$$\boldsymbol{\tau}^R := \mathbf{U}_e 2 \left(\frac{\partial \hat{\psi}}{\partial \mathbf{C}_e} - \frac{\partial \hat{\psi}}{\partial \mathbf{C}_e \otimes \nabla} \cdot \nabla \right) \mathbf{U}_e \tag{2.10}$$

and

$$\mathbf{T}^R := (\mathbf{U}_e \cdot \mathbf{1}_{\mathrm{T}} \cdot \mathbf{U}_e) \cdot\cdot\, 2 \frac{\partial \hat{\psi}}{\partial \mathbf{C}_e \otimes \nabla} \quad , \quad \mathbf{1}_{\mathrm{T}} \cdot\cdot\, \mathbf{A} := \mathbf{A}^{\mathrm{T}} \tag{2.11}$$

as well as the stresses due to the internal state

$$\mathbf{B} := \frac{\partial \hat{\psi}}{\partial \boldsymbol{\alpha} \otimes \nabla} \quad , \quad \mathbf{a} := \frac{\partial \hat{\psi}}{\partial \boldsymbol{\alpha}} - \frac{\partial \hat{\psi}}{\partial \boldsymbol{\alpha} \otimes \nabla} \cdot \nabla \tag{2.12}$$

By inserting eq. (2.5) into (2.9) one gets

$$\begin{aligned} \rho\dot{\psi} = & \left((\dot{\mathbf{F}} \mathbf{F}^{-1})_s \cdot\cdot\, \boldsymbol{\Sigma} J \right) \cdot \nabla + (\dot{\mathbf{F}} \mathbf{F}^{-1})_s \cdot\cdot\, \boldsymbol{\sigma} J \\ & - \left(\mathbf{L}_p^{\mathrm{T}} \cdot\cdot\, \mathbf{S} \right) \cdot \nabla - \mathbf{L}_p^{\mathrm{T}} \cdot\cdot\, \mathbf{M} + (\dot{\boldsymbol{\alpha}} \cdot \mathbf{B}) \cdot \nabla + \dot{\boldsymbol{\alpha}} \cdot \mathbf{a} \end{aligned} \tag{2.13}$$

with the Cauchy stresses

$$\boldsymbol{\sigma} := \tilde{\mathbf{R}} \boldsymbol{\tau}^R \tilde{\mathbf{R}}^{\mathrm{T}} / J \quad , \quad \boldsymbol{\Sigma} := (\tilde{\mathbf{R}} \cdot \mathbf{1}_{\mathrm{T}} \cdot \tilde{\mathbf{R}}) \cdot\cdot\, \mathbf{T}^R / J \quad , \quad J := \det \mathbf{F} \tag{2.14}$$

as well as with the plastic deformation rate $\mathbf{L}_p := \dot{\mathbf{F}}_p \mathbf{F}_p^{-1}$ and the conjugate Mandel stresses

$$\mathbf{M} := \mathbf{U}_e \boldsymbol{\tau}^R \mathbf{U}_e^{-1} = 2 \mathbf{C}_e \left(\frac{\partial \hat{\psi}}{\partial \mathbf{C}_e} - \frac{\partial \hat{\psi}}{\partial \mathbf{C}_e \otimes \nabla} \cdot \nabla \right) \tag{2.15}$$

and

$$\mathbf{S} := (\mathbf{1}_{\mathrm{T}} \cdot \mathbf{U}_e^{-1}) \cdot\cdot (\mathbf{1}_{\mathrm{T}} \cdot \mathbf{U}_e) \cdot\cdot\, \mathbf{T}^R = 2 \mathbf{C}_e \cdot \frac{\partial \hat{\psi}}{\partial \mathbf{C}_e \otimes \nabla} \tag{2.16}$$

The Kirchhoff and the Cauchy stress tensors of second-order (2.10) and (2.14a), respectively, are still symmetric. The Mandel stress of second order (2.15) is generally non-symmetric also for isotropic material behaviour.

Introducing the 1. Piola-Kirchhoff stresses

$$\mathbf{P} := \boldsymbol{\sigma} J \mathbf{F}^{-\mathrm{T}} \quad , \quad \mathbf{T} := (\mathbf{1}_{\mathrm{T}} \cdot \mathbf{F}^{-1}) \cdot\cdot\, \boldsymbol{\Sigma} J \tag{2.17}$$

the rate of strain energy storage (2.13) takes the form

$$\begin{aligned} \rho\dot{\psi} = & \left((\nabla \otimes \dot{\mathbf{u}}) \cdot\cdot\, \mathbf{T} \right) \cdot \nabla + (\nabla \otimes \dot{\mathbf{u}}) \cdot\cdot\, \mathbf{P} \\ & - \left(\mathbf{L}_p : \mathbf{S} \right) \cdot \nabla - \mathbf{L}_p : \mathbf{M} + (\dot{\boldsymbol{\alpha}} \cdot \mathbf{B}) \cdot \nabla + \dot{\boldsymbol{\alpha}} \cdot \mathbf{a} \end{aligned} \tag{2.18}$$

The work done directly on the heterogeneities of the material structure, like the damaging work performed on voids or small cracks, can not be described by the macroscopic displacement field alone. Therefore the power p_b of body forces, not necessarily of external forces $\mathbf{f}$ only, is extended by a term of the macroscopic (stress or strain) quantities working on the internal variables describing the microstructural movement

$$\rho\, p_b = \mathbf{f} \cdot \dot{\mathbf{u}} + \mathbf{y} \cdot \dot{\boldsymbol{\alpha}} \tag{2.19}$$

with an *additional driving force* $\mathbf{y}$ *of the macroscopic loading acting on the substructure*. In this respect the variables $\boldsymbol{\alpha}$ are treated as internal degrees of freedom (Maugin & Muschik, 1994; Sievert et al., 1998; Svendsen, 1999).

Now, with (2.18,19) the dissipation inequality (1.4) can be represented for isothermal processes as

$$\dot{\mathbf{u}}\cdot(\mathbf{f} + \mathbf{P}\cdot\boldsymbol{\nabla} - \rho\ddot{\mathbf{u}}) + (\mathbf{w} - \dot{\mathbf{u}}\cdot\mathbf{P} - (\boldsymbol{\nabla}\otimes\dot{\mathbf{u}})\cdot\cdot\,\mathbf{T} + \mathbf{L}_p:\mathbf{S} - \dot{\boldsymbol{\alpha}}\cdot\mathbf{B})\cdot\boldsymbol{\nabla} \\ + \mathbf{M}:\mathbf{L}_p + (\mathbf{y} - \mathbf{a})\cdot\dot{\boldsymbol{\alpha}} \;\geq\; 0 \tag{2.20}$$

This can be identically fulfilled by

- balance of momentum: $$\mathbf{f} + \mathbf{P}\cdot\boldsymbol{\nabla} = \rho\ddot{\mathbf{u}} \tag{2.21}$$

- power of work at contact: $$\mathbf{w} = \dot{\mathbf{u}}\cdot\mathbf{P} + (\boldsymbol{\nabla}\otimes\dot{\mathbf{u}})\cdot\cdot\,\mathbf{T} - \mathbf{L}_p:\mathbf{S} + \dot{\boldsymbol{\alpha}}\cdot\mathbf{B} \tag{2.22}$$

- residual inequality: $$\rho\, d = \mathbf{M}:\mathbf{L}_p + (\mathbf{y} - \mathbf{a})\cdot\dot{\boldsymbol{\alpha}} \;\geq\; 0 \tag{2.23}$$

The general energy balance (power principle, cf., e.g., Bertram & Forest, 2007) is universal (with a general function for the kinetic energy). But the structure of the quantities within the balances depend generally on the choice of the degrees of freedom for the modelling of the effect of the substructure (a micro-rotation or micro-deformation may be adequate, as discussed in the introduction, or the displacement field alone is sufficient, as assumed in the present paper). Finally, the concrete form of the total stress in the balance, the forms of the power of work at contact and of the power of deformation (see below) have to be consistent with the dependence of the strain energy function on the finite deformation measures. The energy function is considered here as the most fundamental constitutive function (compare Mindlin, 1965, and Trostel, 1985, also for inelastic material behaviour). Thus, in the present theory, the precise forms of the quantities within the balances are calculated straightforward from the dependence of the strain energy function on its independent variables.

With respect to the gradient of displacement term in the work flux (2.22), Mindlin (1965, p. 419) wrote with $\delta\mathbf{u}$ instead of $\dot{\mathbf{u}}$ and without a dyadic product (*S* denotes the surface): "… $\boldsymbol{\nabla}\delta\mathbf{u}$ is not independent of $\delta\mathbf{u}$ on *S* because, if $\delta\mathbf{u}$ is known on *S*, so is the surface-gradient of $\delta\mathbf{u}$.". The reduction of this three-dimensional displacement gradient to the displacement derivative normal to the surface, by means of a divergence theorem on a surface (Brand, 1947) is given for finite deformation by Leroy & Molinari (1993) (compare Sievert, 2001)

$$\mathbf{w}\cdot\mathbf{n} = \dot{\mathbf{u}}\cdot\mathbf{t}_0 + \frac{\partial\dot{\mathbf{u}}}{\partial s_n}\cdot\mathbf{t}_1 - \mathbf{L}_p:\mathbf{S}\cdot\mathbf{n} + \dot{\boldsymbol{\alpha}}\cdot\mathbf{B}\cdot\mathbf{n} \quad , \quad \frac{\partial\dot{\mathbf{u}}}{\partial s_n} := \boldsymbol{\nabla}\cdot\mathbf{n} \tag{2.24}$$

with the boundary stress-vectors

$$\mathbf{t}_0 := \mathbf{P}\cdot\mathbf{n} + (\mathbf{T}\cdot\mathbf{n})\cdot(2H\,\mathbf{n} - \boldsymbol{\nabla}_2) \quad , \quad \boldsymbol{\nabla}_2 := \boldsymbol{\nabla} - \boldsymbol{\nabla}\cdot\mathbf{n}\,\mathbf{n} \quad , \quad 2H := \mathbf{n}\cdot\boldsymbol{\nabla}_2 \tag{2.25a}$$

and

$$\mathbf{t}_1 := (\mathbf{T}\cdot\mathbf{n})\cdot\mathbf{n} \tag{2.25b}$$

$\mathbf{n}$ being the outward unit normal to the surface in the initial placement. The first two terms of the surface power of work (2.24) give the required two vector-valued boundary conditions on each boundary for the partial differential equation (2.21) of fourth order in space for the displacement vector (note $\mathbf{C}_e = \mathbf{F}_p^{-T}\,\mathbf{F}^{T}\,\mathbf{F}\,\mathbf{F}_p^{-1}$). The boundary conditions prescribe either fully the displacement situation, $\mathbf{u}$ and $\dfrac{\partial\mathbf{u}}{\partial s_n}$, or fully the stress state, $\mathbf{t}_0$ and $\mathbf{t}_1$, on the boundary, otherwise mixed boundary conditions are present. The simplest cases are

$$\mathbf{t}_0\big|_b = \mathbf{0} \quad \text{and} \quad \mathbf{t}_1\big|_b = \mathbf{0} \qquad \text{or} \qquad \mathbf{u}\big|_b = \mathbf{0} \quad \text{and} \quad \mathbf{t}_1\big|_b = \mathbf{0} \tag{2.26a,b}$$

But also boundary conditions with a non-vanishing power of work at contact are possible, derived from the evaluation of the dissipation power on the contact surface, see, e.g., Polizotto (2009), Silber et al. (2007).

With eqs. (2.22, 19, 21) the *power of deformation* reads

$$\begin{aligned}&\rho\, p_b - \tfrac{1}{2}\rho\,(\dot{\mathbf{u}}^2)^{\dot{}} + \mathbf{w}\cdot\nabla \;=\\ &(\dot{\mathbf{F}}\,\mathbf{F}^{-1})_{\mathrm{s}}\cdot\cdot\,\boldsymbol{\sigma}\,J + \dot{\boldsymbol{\alpha}}\cdot\mathbf{y} \;+\; \Big((\dot{\mathbf{F}}\,\mathbf{F}^{-1})_{\mathrm{s}}\cdot\cdot\,\boldsymbol{\Sigma}\,J - \mathbf{L}_p : \mathbf{S} + \dot{\boldsymbol{\alpha}}\cdot\mathbf{B}\Big)\cdot\nabla\end{aligned} \tag{2.27}$$

The divergence term on the right hand-side of eq. (2.27) represents a *nonlocal power of deformation of first degree* (compare Edelen & Laws, 1971).

3 Example: Gradients of Elastic and Internal Strains

3.1 Gradients of elastic and plastic strain tensors

3.1.1 Non-symmetric plastic deformation

For $\mathbf{F}_p$ as internal variable $\boldsymbol{\alpha}$ and suppressing, for clarity of the strain gradient theory, classical internal variables

$$\rho\psi = \hat{\psi}\big(\mathbf{C}_e\,,\,\mathbf{C}_e\otimes\nabla,\,\mathbf{F}_p\,,\,\mathbf{F}_p\otimes\nabla\big) \tag{3.1}$$

as well as the additional driving force $\mathbf{y}$, the dissipation inequality (2.23) reads as

$$(\mathbf{M} - \mathbf{X}_p):\mathbf{L}_p \;\geq\; 0 \tag{3.2}$$

with the plastically induced nonlocal back-stress $\mathbf{X}_p$

$$\mathbf{X}_p := \left(\frac{\partial\hat{\psi}}{\partial\mathbf{F}_p} - \frac{\partial\hat{\psi}}{\partial\mathbf{F}_p\otimes\nabla}\cdot\nabla\right)\mathbf{F}_p^{\mathrm{T}} \tag{3.3}$$

(compare Gurtin, 2000). Evaluation of the residual dissipation inequality (3.2) yields the viscoplastic flow rule

$$\dot{\mathbf{F}}_p = \hat{\mathbf{L}}_p(\mathbf{M} - \mathbf{X}_p)\,\mathbf{F}_p \tag{3.4}$$

The power of work at contact (2.24) reads then as

$$\mathbf{w}\cdot\mathbf{n} \;=\; \dot{\mathbf{u}}\cdot\mathbf{t}_0 + \frac{\partial\dot{\mathbf{u}}}{\partial \mathrm{s}_{\mathrm{n}}}\cdot\mathbf{t}_1 \;+\; (\dot{\mathbf{F}}_p\mathbf{F}_p^{-1}):(\mathbf{B}_p - \mathbf{S})\cdot\mathbf{n} \tag{3.5}$$

with the third-order stress tensor $\mathbf{B}_p$

$$\mathbf{B}_p := (\mathbf{1}_{\mathrm{T}}\cdot\mathbf{F}_p)\cdot\cdot\,\mathbf{1}_{\mathrm{T}}\cdot\cdot\frac{\partial\hat{\psi}}{\partial\mathbf{F}_p\otimes\nabla} \tag{3.6}$$

The required boundary condition for the additional partial differential equation (3.4) of second order in space is given by the term $(\dot{\mathbf{F}}_p\mathbf{F}_p^{-1}):(\mathbf{B}_p - \mathbf{S})\cdot\mathbf{n}$ in the surface power of work (3.5). The simplest case is that the higher-order stress $(\mathbf{B}_p - \mathbf{S})\cdot\mathbf{n}$ on the surface of a body vanishes. This is the case if the environment possesses no higher-order stress, i.e. being a pure local material. Even then a plastic strain-rate, $\dot{\mathbf{F}}_p\mathbf{F}_p^{-1}$, can be present on the surface of a body. The other type of boundary conditions is generally that the conjugate strain-rate, here $\dot{\mathbf{F}}_p\mathbf{F}_p^{-1}$, is prescribed, for example as zero, if physically reasonable. In this case of a kinematical boundary condition, a non-vanishing higher-order stress $(\mathbf{B}_p - \mathbf{S})\cdot\mathbf{n}$ can exist on the surface of the body resulting from the vanishing of the plastic strain-rate on the surface.

For more advanced boundary conditions without an elastic strain gradient and thus without $\mathbf{S}$, see Gurtin & Needleman (2005).

Strain gradient models for viscoelastic materials were given by Sievert (2001) based on the Burgers model using a multiplicative decomposition of the plastic deformation $\mathbf{F}_p$ into a Kelvin-Voigt- and a Maxwell-type deformation according to Sidoroff (1976), taking also into account energy storage due the spatial gradients of these deformation parts and evaluating the dissipation inequality as shown above. An alternative gradient-approach to viscoelasticity has been proposed by Saczuk et al. (2003) without using an elastic-inelastic decomposition of deformation as eq. (2.1).

The free energy of the present second gradient theory is a function of a third-order tensor so that the representations of the isotropic functions of such tensors given by Silber (1990) could be useful.

Like the entire local deformation $\mathbf{F}$, the plastic deformation $\mathbf{F}_p$ can also be decomposed into a pure rotation $\mathbf{R}_p$ and a plastic stretch $\mathbf{U}_p$: $\mathbf{F}_p = \mathbf{R}_p\, \mathbf{U}_p$. The orthogonal tensor of a polar decomposition describes generally the rotation of the principal directions of the stretch tensor. As mentioned above, for anisotropic materials the generally non-symmetric tensor $\mathbf{F}_p$ describes the plastic deformation of a material element with respect to the material directions. Therefore, $\mathbf{R}_p$ describes the plastic rotation of the principal directions of the plastic stretch $\mathbf{U}_p$ with respect to the material directions and thus, conversely, $\mathbf{R}_p$ describes also the rotation of the material directions relative to the principal directions of the plastic stretch $\mathbf{U}_p$ due to the plastic deformation $\mathbf{F}_p$ of the material element.

3.1.2 Straining described by stretch tensors

If initially isotropic materials are considered and texture development, if significant, may be approximated by the plastic stretch $\mathbf{U}_p$ itself or if material directions are completely deforming as line-elements of the macroscopic continuum element, then the entire plastic deformation of a material element is described by the plastic stretch alone (Mandel, 1974, p. 292; compare Rice, 1975, p. 25, 30)

$$\mathbf{F}_p \equiv \mathbf{U}_p \quad \Leftrightarrow \quad \mathbf{R}_p \equiv \mathbf{1} \tag{3.7}$$

and the physical plastic rotation $\mathbf{R}_p$ vanishes[1] $\mathbf{F} = \tilde{\mathbf{R}}\, \mathbf{U}_e\, \mathbf{U}_p$ (Haupt, 1984).

The rate of the elastic Cauchy-Green tensor $\mathbf{C}_e := \mathbf{U}_e^2$ is then according to eqs. (2.6, 5)

$$\dot{\mathbf{C}}_e = \mathbf{U}_e 2(\mathbf{D}^R - \mathbf{D}_p^R)\, \mathbf{U}_e \quad , \quad \mathbf{D}^R := \tilde{\mathbf{R}}^{\mathrm{T}} \big(\dot{\mathbf{F}}\,\mathbf{F}^{-1}\big)_{\mathrm{s}}\, \tilde{\mathbf{R}} \quad , \quad \mathbf{D}_p^R := (\mathbf{U}_e \dot{\mathbf{U}}_p \mathbf{U}_p^{-1} \mathbf{U}_e^{-1})_{\mathrm{s}} \tag{3.8}$$

In order to model the influence of plastic strain gradients on the material behaviour at finite deformation reference will be made to the description of hardening. For the modelling of the *Bauschinger effect* at finite strain, an internal strain tensor induced by viscoplastic straining could be introduced (compare, e.g., Dogui & Sidoroff, 1985; Svendsen et al., 1998; Wallin & Ristinmaa, 2005), by which energy due to hardening, so-called latent energy (Freudenthal, 1950, p. 275; Taylor & Quinney, 1934), is stored. Analogously to the evolution equation (3.8) for the elastic strain $\mathbf{C}_e$, an internal strain tensor, called *latent strain* $\mathbf{C}_l =: \mathbf{U}_l^2$, can be defined by the evolution equation

$$\dot{\mathbf{C}}_l = \mathbf{U}_l\, 2(\mathbf{D}_p^R - \mathbf{D}_i^R)\, \mathbf{U}_l \tag{3.9}$$

[1] On the basis of eq. (2.1) the Green strain tensor has in general an additive elastic-plastic decomposition

$$\tfrac{1}{2}(\mathbf{C}-\mathbf{1}) = \tfrac{1}{2}\big(\mathbf{F}_p^{\mathrm{T}} \mathbf{U}_e^2\, \mathbf{F}_p - \mathbf{1}\big) = \mathbf{F}_p^{\mathrm{T}}\, \tfrac{1}{2}(\mathbf{U}_e^2 - \mathbf{1})\, \mathbf{F}_p + \tfrac{1}{2}(\mathbf{F}_p^{\mathrm{T}}\mathbf{F}_p - \mathbf{1}) \quad , \quad \mathbf{C} := \mathbf{F}^{\mathrm{T}}\,\mathbf{F}$$

similar to the one of Green & Naghdi (1965). The plastic strain tensor $\tfrac{1}{2}(\mathbf{F}_p^{\mathrm{T}}\mathbf{F}_p - \mathbf{1})$ is under the assumption (3.7) equivalent to the, then, total plastic deformation $\mathbf{U}_p$ (compare Green & Naghdi, 1971).

with the viscoplastic strain-rate $\mathbf{D}_p^R$ instead of the total strain-rate $\mathbf{D}^R$ of eq. (3.8)a and an observer-invariant recovery strain-rate $\mathbf{D}_i^R$ instead of the viscoplastic strain-rate of eq. (3.8)a. The strain $\frac{1}{2}(\mathbf{C}_l - \mathbf{1})$ is just the finite deformation generalisation of the well-known strain-like kinematic hardening variable ($\boldsymbol{\alpha}$) for small deformations (Lemaitre & Chaboche, 1990).

Introducing the latent strain $\mathbf{C}_l$ as internal variable $\boldsymbol{\alpha}$ with the evolution equation (3.9)

$$\rho\psi = \hat{\psi}\left(\mathbf{C}_e, \mathbf{C}_e\otimes\nabla, \mathbf{C}_l, \mathbf{C}_l\otimes\nabla\right) \tag{3.10}$$

and still suppressing an additional driving force $\mathbf{y}$, the dissipation inequality (2.23) reads, with the Mandel stress $\mathbf{M}$ according to eq. (2.15) and with the back-rotated Kirchhoff stress $\boldsymbol{\tau}^R$ according to eq. (2.10), as

$$\rho\, d = (\boldsymbol{\tau}^R - \mathbf{X})\cdot\cdot\,\mathbf{D}_p^R + \mathbf{X}\cdot\cdot\,\mathbf{D}_i^R \geq 0 \tag{3.11}$$

together with the also symmetric, plastically induced nonlocal back-stress $\mathbf{X}$

$$\mathbf{X} := \mathbf{U}_l\, 2\left(\frac{\partial\hat{\psi}}{\partial\mathbf{C}_l} - \frac{\partial\hat{\psi}}{\partial\mathbf{C}_l\otimes\nabla}\cdot\nabla\right)\mathbf{U}_l \tag{3.12}$$

which has a structure similar to the one of the back-rotated Kirchhoff stress of eq. (2.10).

The residual dissipation inequality (3.11) can be identically fulfilled by flow rules for the viscoplastic strain-rate $\mathbf{D}_p^R$

$$\mathbf{D}_p^R = \hat{\mathbf{D}}_p^R(\boldsymbol{\tau}^R - \mathbf{X}) \tag{3.13)a}$$

and for the recovery strain-rate $\mathbf{D}_i^R$

$$\mathbf{D}_i^R = \boldsymbol{f}(\mathbf{X})\,\dot{p} + \boldsymbol{g}(\mathbf{X}) \tag{3.13)b}$$

with so-called dynamic and static recovery terms (e.g., Chaboche, 1997) with the functions $\boldsymbol{f}$ and $\boldsymbol{g}$, respectively. It is assumed that the nonlinear constitutive function $\hat{\mathbf{D}}_p^R$ fulfills the condition $(\boldsymbol{\tau}^R - \mathbf{X})\cdot\cdot\,\hat{\mathbf{D}}_p^R(\boldsymbol{\tau}^R - \mathbf{X}) \geq 0$. The recovery functions $\boldsymbol{f}$ and $\boldsymbol{g}$ satisfy the conditions $\mathbf{X}\cdot\cdot\,\boldsymbol{f}(\mathbf{X}) \geq 0$ and $\mathbf{X}\cdot\cdot\,\boldsymbol{g}(\mathbf{X}) \geq 0$. $\dot{p}$ is an equivalent plastic strain-rate which is homogeneously in the magnitude $\left\|\mathbf{D}_p^R\right\|$, with $\dot{p} > 0$ if $\left\|\mathbf{D}_p^R\right\| > 0$.

For example, the tensor-linear flow rule reads as

$$\hat{\mathbf{D}}_p^R(\boldsymbol{\tau}^R - \mathbf{X}) \equiv \hat{\mathrm{f}}(\boldsymbol{\tau}^R - \mathbf{X})\; \mathbf{A}\cdot\cdot(\boldsymbol{\tau}^R - \mathbf{X}) \tag{3.14}$$

with a scalar nonlinear function $\hat{\mathrm{f}}$, the fourth-order constitutive tensor $\mathbf{A}$ fulfills the condition $(\boldsymbol{\tau}^R - \mathbf{X})\cdot\cdot\,\mathbf{A}\cdot\cdot(\boldsymbol{\tau}^R - \mathbf{X}) \geq 0$. The tensor-linear examples for the dynamic and static recovery function $\boldsymbol{f}$ and $\boldsymbol{g}$, respectively, are given by Nouailhas & Freed (1992) for small strain and pure local constitutive modelling, but this can be applied directly to the flow rule (3.13)b for the recovery strain-rate $\mathbf{D}_i^R$.

Equations (2.21), (3.13)a with (3.8)c and (3.9) with (3.13)b are three coupled partial differential equations of fourth order in space for the displacement $\mathbf{u}$ and of second order in space for $\mathbf{U}_p$ and $\mathbf{C}_l$, due to the second spatial derivative of the elastic strain $\mathbf{C}_e = \mathbf{U}_p^{-\mathrm{T}}\,\mathbf{F}^{\mathrm{T}}\,\mathbf{F}\,\mathbf{U}_p^{-1}$ in the Kirchhoff stress $\boldsymbol{\tau}^R$ according to eq. (2.10)a and of the latent strain $\mathbf{C}_l$ in the nonlocal back-stress $\mathbf{X}$ (3.12), respectively.

Eq. (3.9) can be re-written as

$$\mathbf{D}_p^R = \mathbf{D}_l^R + \mathbf{D}_i^R \qquad , \qquad \mathbf{D}_l^R := \mathbf{U}_l^{-1}\, \tfrac{1}{2}\dot{\mathbf{C}}_l\, \mathbf{U}_l^{-1} \tag{3.15}$$

For a polymer the strain-rate $\mathbf{D}_l^R$ describes the time-dependent stretching of the polymer chains (Kelvin-Voigt-type deformation) and the inelastic strain-rate $\mathbf{D}_i^R$ represents the changing of the junctions between the chains (Maxwell-type deformation, see, e.g., Giesekus, 1994, p. 272; a non-symmetric Maxwell deformation tensor is considered in Sievert, 2001).

Inserting the decomposition (3.15) of the total inelastic strain-rate $\mathbf{D}_p^R$ into the dissipation inequality (3.11)

$$(\boldsymbol{\tau}^R - \mathbf{X}) \cdot\cdot\, \mathbf{D}_l^R + \boldsymbol{\tau}^R \cdot\cdot\, \mathbf{D}_i^R \geq 0 \tag{3.16}$$

and evaluating the latter with respect to the Kelvin-type strain-rate $\mathbf{D}_l^R$ and the Maxwell-type strain-rate $\mathbf{D}_i^R$, in order to achieve nonlinear flow rules for these strain-rates in dependence on the conjugate stresses, $\mathbf{D}_l^R = \hat{\mathbf{D}}_l^R(\boldsymbol{\tau}^R - \mathbf{X})$ and $\mathbf{D}_i^R = \hat{\mathbf{D}}_i^R(\boldsymbol{\tau}^R)$, then one has for a viscoelastic material via (3.15)a with (3.8)c and via (3.15)b evolution equations for $\mathbf{U}_p$ and $\mathbf{C}_l$, respectively, two coupled partial differential equations of second order in space in these variables.

Special constitutive equations for viscoelastic materials have been given by Sievert (2001) considering energy storage with gradients only of scalar quantities as the volumetric elastic stretch, the magnitude of an isochoric elastic stretch tensor as well as an accumulated inelastic strain. The representations of the stresses depending on the gradients of these scalar elastic quantities are given in appendix B and the evaluation of the dissipation inequality with respect to an accumulated inelastic strain is carried out in the next section.

The power of work at contact (2.24) for the variables of the present section reads as

$$\mathbf{w} \cdot \mathbf{n} = \dot{\mathbf{u}} \cdot \mathbf{t}_0 + \frac{\partial \dot{\mathbf{u}}}{\partial s_n} \cdot \mathbf{t}_1 - \mathbf{D}_p^R \cdot\cdot\, \mathbf{T}^R \cdot \mathbf{n} + \dot{\mathbf{C}}_l \cdot\cdot\, \mathbf{B}_l \cdot \mathbf{n} \tag{3.17}$$

with the higher-order stress tensor $\mathbf{T}^R$ according to eq. (2.11) and the residual stress tensor $\mathbf{B}_l$ due to the gradient of the latent strain $\mathbf{C}_l$

$$\mathbf{B}_l := \frac{\partial \hat{\psi}}{\partial \mathbf{C}_l \otimes \nabla} \tag{3.18}$$

The required boundary conditions for the two additional partial differential equations are given by the last two terms in the surface power of work (3.17). The simplest case is that the higher-order stresses $\mathbf{B}_l \cdot \mathbf{n}$ and $\mathbf{T}^R \cdot \mathbf{n}$ on the surface of a body vanish.

The power of deformation reads

$$\begin{aligned} &\rho\, p_b - \tfrac{1}{2}\rho\, (\dot{\mathbf{u}}^2)^{\cdot} + \mathbf{w} \cdot \nabla = \\ &(\dot{\mathbf{F}}\,\mathbf{F}^{-1})_s \cdot\cdot\, \boldsymbol{\sigma} J + \left((\dot{\mathbf{F}}\,\mathbf{F}^{-1})_s \cdot\cdot\, \boldsymbol{\Sigma} J - \mathbf{D}_p^R \cdot\cdot\, \mathbf{T}^R + \dot{\mathbf{C}}_l \cdot\cdot\, \mathbf{B}_l \right) \cdot \nabla \end{aligned} \tag{3.19}$$

3.2 Gradient of elastic and accumulated viscoplastic strain

For the case of the scalar internal variable of an accumulated viscoplastic strain p by which spatial gradient energy is stored

$$\rho\psi = \hat{\psi}\left(\mathbf{C}_e, \mathbf{C}_e \otimes \nabla, p, \nabla p\right) \tag{3.20}$$

the dissipation inequality (2.23) reads with (2.12)b, still without an additional driving force **y**, as

$$\boldsymbol{\tau}^R \cdot\cdot \mathbf{D}_p^R - \left(\frac{\partial \hat{\psi}}{\partial p} - \frac{\partial \hat{\psi}}{\partial \nabla p} \cdot \nabla \right) \dot{p} \;\geq\; 0 \tag{3.21}$$

With a related plastic strain-rate $\vec{\mathbf{D}}_p^R$, eq. (3.21) can be expressed as

$$\left(\boldsymbol{\tau}^R \cdot\cdot \vec{\mathbf{D}}_p^R - \left(\frac{\partial \hat{\psi}}{\partial p} - \frac{\partial \hat{\psi}}{\partial \nabla p} \cdot \nabla \right) \right) \dot{p} \;\geq\; 0 \quad , \quad \vec{\mathbf{D}}_p^R := \mathbf{D}_p^R / \dot{p} \tag{3.22}$$

Now, with a flow rule for the related plastic strain-rate

$$\vec{\mathbf{D}}_p^R = \hat{\vec{\mathbf{D}}}_p^R \left(\boldsymbol{\tau}^R \right) \tag{3.23}$$

and assuming $\boldsymbol{\tau}^R \cdot\cdot \hat{\vec{\mathbf{D}}}_p^R \geq 0$, eq. (3.22) can be re-written with an equivalent stress σ_{eq} as

$$\left(\sigma_{\text{eq}} - \left(\frac{\partial \hat{\psi}}{\partial p} - \frac{\partial \hat{\psi}}{\partial \nabla p} \cdot \nabla \right) \right) \dot{p} \;\geq\; 0 \quad , \quad \sigma_{\text{eq}} := \boldsymbol{\tau}^R \cdot\cdot \hat{\vec{\mathbf{D}}}_p^R \tag{3.24}$$

This inequality can be identically fulfilled for viscoplastic material behaviour by the flow rule

$$\begin{aligned} &\dot{p} = f\left(\sigma_{\text{eq}} - \left(\frac{\partial \hat{\psi}}{\partial p} - \frac{\partial \hat{\psi}}{\partial \nabla p} \cdot \nabla \right), \, p \right) \\ &\qquad \text{if } \sigma_{\text{eq}} - \left(\frac{\partial \hat{\psi}}{\partial p} - \frac{\partial \hat{\psi}}{\partial \nabla p} \cdot \nabla \right) > 0 \quad , \quad \dot{p} = 0 \text{ otherwise} \end{aligned} \tag{3.25}$$

with a nonlinear function *f*.

The flow rule for the entire plastic strain-rate reads according to eq. (3.22)b with eq. (3.23) as

$$\mathbf{D}_p^R = \dot{p}\; \hat{\vec{\mathbf{D}}}_p^R \left(\boldsymbol{\tau}^R \right) \tag{3.26}$$

The power of work at contact (2.24) is

$$\mathbf{w} \cdot \mathbf{n} = \dot{\mathbf{u}} \cdot \mathbf{t}_0 + \frac{\partial \dot{\mathbf{u}}}{\partial \mathrm{s}_\mathrm{n}} \cdot \mathbf{t}_1 - \mathbf{D}_p^R \cdot\cdot \mathbf{T}^R \cdot \mathbf{n} + \dot{p}\, \mathbf{b}_p \cdot \mathbf{n} \tag{3.27}$$

with the residual stress vector

$$\mathbf{b}_p := \frac{\partial \hat{\psi}}{\partial \nabla p} \quad . \tag{3.28}$$

The required boundary conditions for the two coupled additional partial differential equations (3.25) and (3.26) with (3.8)c for p and $\mathbf{U}_p$ are given by the last two terms in the surface power of work (3.27). The simplest case is that the higher-order stresses $\mathbf{b}_p \cdot \mathbf{n}$ and $\mathbf{T}^R \cdot \mathbf{n}$ on the surface of a body vanish.

Energy storage with the gradient of a scalar variable, such as p, is also for cubic material symmetry isotropic. This leads for a quadratic form, besides energy storage with $\mathbf{C}_e$, to

$$\rho\psi = \hat{\psi}(\mathbf{C}_e, \nabla p) \equiv \tfrac{1}{2} \hat{\mathrm{W}}_e(\mathbf{C}_e) + \tfrac{1}{2} \mathrm{k}\,(\nabla p)^2 \tag{3.29}$$

Then the plasticity induced residual stress vector $\mathbf{b}_p$ reads as

$$\mathbf{b}_p := \frac{\partial \hat{\psi}}{\partial \nabla p} \equiv \mathrm{k}\, \nabla p \tag{3.30}$$

If the stiffness k would be a function, for example of the accumulated plastic strain, then the divergence-derivative in eq. (3.21) would have to be applied also to that. But k is assumed as constant here. Therefore the flow rule (3.25) yields the form

$$\dot{p} = f\left(\sigma_{\mathrm{eq}} + \mathrm{k}\, \Delta p, p\right) \quad \text{if} \ \ \sigma_{\mathrm{eq}} + \mathrm{k}\, \Delta p > 0 \quad , \quad \dot{p} = 0 \ \text{otherwise} \tag{3.31}$$

$\Delta := \nabla \cdot \nabla$ denotes the Laplace operator. The second derivative of the plastic strain p is negative in the centre of localization, e.g. of a shear band. Thereby the Laplace-term in (3.31) acts as a back-stress and delocalises in this way the p-field.

Inverting the flow rule (3.31), the equivalent stress can be represented as

$$\sigma_{\mathrm{eq}} = \kappa_p(\dot{p}, p) - \mathrm{k}\, \Delta p \quad \text{if} \quad \dot{p} > 0 \quad , \quad \kappa_p(\dot{p}, p) := f^{-1}(\dot{p}; p) \tag{3.32}$$

With the equivalent Mises strain-rate $\dot{p} \equiv \sqrt{\tfrac{2}{3}} \left\| \mathbf{D}_p^R \right\|$ and with the rule $\hat{\mathbf{D}}_p^R \equiv \sqrt{\tfrac{3}{2}}\, \boldsymbol{\tau}^{R'} / \left\| \boldsymbol{\tau}^{R'} \right\|$ for the direction of isochoric plastic flow of an isotropic material ($\boldsymbol{\tau}^{R'}$ being the stress deviator), eq. (3.24)b for the equivalent stress yields the Mises stress $\sigma_{\mathrm{eq}} \equiv \sqrt{\tfrac{3}{2}} \left\| \boldsymbol{\tau}^{R'} \right\|$ (for anisotropic materials with the Hill stress as equivalent stress, see Nouailhas & Freed, 1992). The derivation of eq. (3.32) represents a thermodynamical foundation of the viscoplastic flow rule of Zbib & Aifantis (1988).

A vanishing of the higher stress $\mathbf{b}_p \cdot \mathbf{n}$ on the surface of a body means because of the linear relationship (3.30) that the derivative of the accumulated plastic strain p normal to the surface is zero $\partial p / \partial \mathrm{n} := \mathbf{n} \cdot \nabla p = 0$.

The so-called implicit gradient-enhanced approach to elastoplasticity (Peerlings et al., 2001; Engelen et al., 2003) introduces a linear equation between the difference of the accumulated plastic strain and an additional internal degree of freedom $\bar{p}$ on the one hand, and the Laplace operator of that additional degree of freedom on the other hand

$$-\frac{\mathrm{k}}{\mathrm{h}} \Delta \bar{p} = p - \bar{p} \tag{3.33}$$

Such a relation has been discovered by Forest (2009) as the micro-strain balance of a special case of the thermodynamically consistent micromorphic theory with a general formulation of the boundary conditions. In the micromorphic context not only a softening variable can be delocalised, but via the difference between the macro- and the micro-strain $\mathrm{h}\left(p - \bar{p}\right)$, which enters as a backstress in the flow rule, also hardening due to inhomogeneous deformation can be described by the Laplace derivation of that additional degree of freedom, similar to the Aifantis equation (3.31), and that without any softening variable. The additional degree of freedom is not restricted to be a scalar but it can be any tensorial variable (Forest, 2009). For finite deformations viscoplastic micromorphic theories have been given by Forest & Sievert (2003, 2006).

Of course, a micromorphic model contains at least one additional material parameter (h) related to the micro-field. But even due to this freedom the micromorphic theory offers an interesting approach for the numerical implementation of gradient plasticity models by imposing an internal constraint on the difference variable between the macroscopic and the micromorphic field via penalising the departure of the micro-variable from the macro-variable by the related stiffness (h) which then becomes a Lagrange multiplier (Forest, 2009, p. 129; compare Cordero et al., 2010). Hence, the micro-variable follows the macro-variable and, for example, also the Laplace operator of the additional degree of freedom $\bar{p}$ mentioned above becomes the Laplace derivation of the macroscopic accumulated plastic strain p, and therewith the nonlocal flow rule (3.31) is implemented, but using the linear partial differential equation (3.33), which is numerically more easy to handle.

4 Example: Gradient-dependent Damage

4.1 Derivation of the damage evolution equation

For the case of a scalar damage variable s by which spatial gradient energy is stored

$$\rho\psi = \hat{\psi}\left(\mathbf{C}_e , \mathbf{C}_e \otimes \nabla , s , \nabla s\right) \tag{4.1}$$

the dissipation inequality (2.23) reads with (2.12)b as

$$\rho d = \boldsymbol{\tau}^R \cdot\cdot \mathbf{D}_p^R + \left(\mathrm{y} - \left(\frac{\partial\hat{\psi}}{\partial s} - \frac{\partial\hat{\psi}}{\partial \nabla s} \cdot \nabla \right) \right) \dot{s} \geq 0 \tag{4.2}$$

with an additional damage driving force y of the macroscopic loading acting on defects that will be specified below.

Damage evolution is essentially divided into two time-phases: the growth of single defects (voids, small cracks) and the phase of defects growing together. Under cyclic loading (growth of small cracks) the first phase often has essentially no influence on the macroscopic stress-strain behaviour, in the second time-phase there is an influence on it. The evolution equation is formulated here primarily for an internal time variable s, ranging from 0 to 1, scaling the whole lifetime. The effect of damage D on the macroscopically applied stress arises, according to Lemaitre (1985), via the decreasing load bearing capacity 1-D of a cross section of a material element. Macroscopic damage (D) occurs under cyclic loading often close to total failure of a material element. Then D becomes significant shortly before $s = 1$. Thus, D is a strong nonlinear function of the lifetime variable s, for example, in a compact form: $\mathrm{D} = s^{\mathrm{r}}$, r » 1.

The residual inequality (4.2) can be identically fulfilled with respect to the damage by the evolution equation

$$\mathrm{c}\,\dot{s} = \left(\mathrm{y} - \left(\frac{\partial\hat{\psi}}{\partial s} - \frac{\partial\hat{\psi}}{\partial \nabla s} \cdot \nabla \right) \right) \dot{p} \tag{4.3}$$

where $\dot{p}$ represents an equivalent plastic strain-rate.

Quadratic energy storage with the gradient of the internal time variable s is for an isotropic or cubic material, besides energy storage with $\mathbf{C}_e$, represented by

$$\rho\psi = \hat{\psi}(\mathbf{C}_e, s, \nabla s) \equiv \tfrac{1}{2}(1-\mathrm{D}(s))\, \hat{\mathrm{W}}_e(\mathbf{C}_e - \mathbf{1}) + \tfrac{1}{2}\mathrm{k}\,(\nabla s)^2 \quad , \quad \mathrm{D}(s) = s^{\mathrm{r}} \tag{4.4}$$

with the dependence of the elastic energy on damage according to Lemaitre (1985). Then the damage induced residual stress vector $\mathbf{b}_s$ reads as

$$\mathbf{b}_s := \frac{\partial\hat{\psi}}{\partial \nabla s} \equiv \mathrm{k}\,\nabla s \tag{4.5}$$

and the evolution equation (4.3) becomes for a constant gradient stiffness k

$$\mathrm{c}\,\dot{s} = \left(\mathrm{y} - \frac{\partial\hat{\psi}}{\partial s} + \mathrm{k}\,\Delta s \right) \dot{p} \tag{4.6}$$

(Sievert et al., 1998). The required boundary condition for this evolution equation as an additional partial differential equation is given by the last term of the power of work at contact (2.24). The simplest case is again to assume that the higher stress $\mathbf{b}_s \cdot \mathbf{n}$ vanishes on the surface of a body.

4.2 Rate-dependent damage

Assuming in (4.6) $\mathrm{c} \equiv \mathrm{W_c}\, \dot{p}$, a rate-dependent evolution equation results

$$\mathrm{W_c}\, \dot{s} \;=\; \mathrm{y} - \frac{\partial \hat{\psi}}{\partial s} \;+\; \mathrm{k}\, \Delta s \tag{4.7}$$

For y≡0 and r=1, i.e. $\mathrm{D} \equiv s$, this is via (4.3) the gradient-dependent evolution equation

$$\mathrm{W_c}\, \dot{s} \;=\; \mathrm{W}_e \;+\; \mathrm{k}\, \Delta s \tag{4.8}$$

of Maugin (1990, eq. $(8.14)_5$). Damage, especially material separation, was observed in a metal also at high strain-rates ($\geq 10^3$ 1/s; Sievert et al., 2003). Therefore, damage should arise in the model also at a much faster plastic deformation, thus the damage evolution equation should be homogeneously in the plastic strain-rate.

For $\dfrac{\partial \hat{\psi}}{\partial s} \equiv 0$ and $\mathrm{y} \equiv \dfrac{\sigma_{\mathrm{eq}}}{1-\mathrm{D}}\, \dot{p}$ with an equivalent stress σ_{eq}, eq. (4.7) yields

$$\mathrm{W_c}\, \dot{s} \;=\; \frac{\sigma_{\mathrm{eq}}}{1-\mathrm{D}}\, \dot{p} \;+\; \mathrm{k}\, \Delta s \tag{4.9}$$

an evolution equation similar to the rate-dependent damage model of Reusch et al. (2003a). The material constant $\mathrm{W_c}$ represents a critical plastic work to be reached for total failure. With increasing plastic strain rate $\dot{p}$ the delocalisation effect due to the Laplace-term in eq. (4.9) vanishes for a constant stiffness k (compare Sievert & Kiyak, 2005). If k would be a constitutive function then the divergence in eq. (4.3) must be applied also to k. Therefore the following way is pursued for the description of damage localisation also at higher plastic strain rates.

4.3 Fully plastic strain controlled damage

For $\mathrm{c} = \mathrm{W_c}$, $\dfrac{\partial \hat{\psi}}{\partial s} \equiv 0$ and the effective stress $\mathrm{y} \equiv \dfrac{\sigma_{\mathrm{eq}}}{1-\mathrm{D}}$ as driving stress, eq. (4.6) yields

$$\mathrm{W_c}\, \dot{s} \;=\; \left(\frac{\sigma_{\mathrm{eq}}}{1-\mathrm{D}} \;+\; \mathrm{k}\, \Delta s \right) \dot{p} \quad . \tag{4.10}$$

Due to the proportionality of this equation to the equivalent plastic strain-rate $\dot{p}$, the damage evolution is fully controlled by the plastic strain. For rate-independent stress-strain behaviour, an exactly rate-independent evolution results according to eq. (4.10). Eqs. (4.9) and (4.10) will be investigated in sect. 5.

If one takes into account in the dissipation inequality (3.21) for the consideration of the gradient of accumulated viscoplastic strain an additional driving force $\mathrm{y} \equiv \sigma_{\mathrm{eq,eff}} - \sigma_{\mathrm{eq}}$ as in eq. (4.2), then the equivalent stress σ_{eq} in eq. (3.25) can be replaced via $\sigma_{\mathrm{eq}} + \mathrm{y} \equiv \sigma_{\mathrm{eq,eff}}$ by the effective stress $\sigma_{\mathrm{eq,eff}} := \sigma_{\mathrm{eq}} /(1-\mathrm{D})$, and thus, the gradient-dependent flow rule (3.25) can also be used for a damaged material

$$\begin{aligned} \dot{p} &= f\left(\sigma_{\mathrm{eq,eff}} - \left(\frac{\partial \hat{\psi}}{\partial p} - \frac{\partial \hat{\psi}}{\partial \nabla p} \cdot \nabla \right),\, p \right) \\ &\quad \text{if } \sigma_{\mathrm{eq,eff}} - \left(\frac{\partial \hat{\psi}}{\partial p} - \frac{\partial \hat{\psi}}{\partial \nabla p} \cdot \nabla \right) > 0 \quad , \quad \dot{p} = 0 \text{ otherwise} \end{aligned} \tag{4.12}$$

5 Comparison of Two Gradient-Dependent Damage Models at a Crack Tip

5.1 Isotropic local constitutive stress-strain relations at small elastic strain

At first the constitutive stress-strain relations shall be specialized. As indicated in sect. 3.2, the orthogonal part $\mathbf{R}_p$ of the plastic deformation $\mathbf{F}_p$ describes also the rotation of the material directions relative to the principal directions of the plastic stretch $\mathbf{U}_p$ due to the plastic deformation $\mathbf{F}_p$ of the material element. If no material directions are present, then the entire plastic deformation of a material element is described by the plastic stretch alone, $\mathbf{F}_p \equiv \mathbf{U}_p$, and the plastic rotation $\mathbf{R}_p$ vanishes: $\mathbf{R}_p \equiv \mathbf{1}$.

At small elastic strain, $\mathbf{U}_e = \mathbf{1} + \boldsymbol{\varepsilon}_e$, $\|\boldsymbol{\varepsilon}_e\| \ll 1$, products including the small elastic strain $\boldsymbol{\varepsilon}_e$ can be neglected with respect to products with $\mathbf{1}$

$$\mathbf{F} = \tilde{\mathbf{R}}\,\mathbf{U}_e\,\mathbf{F}_p \equiv \tilde{\mathbf{R}}\,\mathbf{U}_e\,\mathbf{U}_p \approx \tilde{\mathbf{R}}\,\mathbf{U}_p \approx \mathbf{R}\,\mathbf{U} \tag{5.1}$$

One observes that the rigid rotation $\tilde{\mathbf{R}}$ of a material element can then be identified with the rotation $\mathbf{R}$ of the polar decomposition of $\mathbf{F}$: $\tilde{\mathbf{R}} \approx \mathbf{R}$ (compare Haupt, 1985).

The evolution equation for the small elastic strain $\boldsymbol{\varepsilon}_e$ results directly from eq. (5.1) by material time derivation[2]:

$$\dot{\boldsymbol{\varepsilon}}_e \approx (\dot{\mathbf{U}}_e\mathbf{U}_e^{-1})_s = \mathbf{D}^R - \mathbf{D}_p^R \tag{5.2a}$$

$$\mathbf{D}^R := \tilde{\mathbf{R}}^T\mathbf{D}\,\tilde{\mathbf{R}} \approx \mathbf{R}^T\mathbf{D}\,\mathbf{R} \equiv \left(\dot{\mathbf{U}}\,\mathbf{U}^{-1}\right)_s \equiv 1/2\,\mathbf{U}^{-1}\dot{\mathbf{C}}\,\mathbf{U}^{-1}$$
$$\mathbf{D} := \left(\dot{\mathbf{F}}\,\mathbf{F}^{-1}\right)_s \quad , \quad \mathbf{C} := \mathbf{F}^T\mathbf{F} \equiv \mathbf{U}^2 \tag{5.2b,c,d}$$

$$\mathbf{D}_p^R := (\mathbf{U}_e\dot{\mathbf{U}}_p\mathbf{U}_p^{-1}\mathbf{U}_e^{-1})_s \approx (\dot{\mathbf{U}}_p\mathbf{U}_p^{-1})_s \tag{5.2e}$$

At no energy storage with the gradient of the elastic strain, the Mandel stress is according to eq. (2.15) for an elastically isotropic material equal to the back-rotated Kirchhoff stress $\boldsymbol{\tau}^R$ and thus symmetric

$$\mathbf{M} \equiv \boldsymbol{\tau}^R := \boldsymbol{\sigma}^R J \equiv \mathbf{U}_e 2\frac{\partial\hat{\psi}}{\partial\mathbf{C}_e}\mathbf{U}_e \approx \frac{\partial\hat{\psi}}{\partial\boldsymbol{\varepsilon}_e} \tag{5.3}$$

The constitutive modelling (5.1) and (5.3) is assumed in the next section.

At small latent strain, $\mathbf{U}_l = \mathbf{1} + \boldsymbol{\varepsilon}_l$, $\|\boldsymbol{\varepsilon}_l\| \ll 1$, eq. (3.12) leads with the evolution equation (3.9), for isotropic material behaviour and for quadratic energy storage with a deviatoric strain tensor $\boldsymbol{\varepsilon}_l$ (stiffness k) and no energy storage with its gradient, to the classical kinematic hardening rule

$$\dot{\mathbf{X}} = \frac{d\hat{\mathbf{X}}}{d\mathbf{C}_l}\cdot\cdot\,\dot{\mathbf{C}}_l \approx k\,(\mathbf{D}_p^R - \mathbf{D}_i^R) \tag{5.4}$$

---

[2] The spin tensor of the deformation-rate $\dot{\mathbf{F}}\mathbf{F}^{-1}$ is on the basis of eq. (5.1) for small elastic strain represented by

$$\begin{aligned}
(\dot{\mathbf{F}}\mathbf{F}^{-1})_{skw} &= \dot{\tilde{\mathbf{R}}}\tilde{\mathbf{R}}^T + \tilde{\mathbf{R}}(\dot{\mathbf{U}}_e\mathbf{U}_e^{-1})_{skw}\tilde{\mathbf{R}}^T + \tilde{\mathbf{R}}(\mathbf{U}_e\dot{\mathbf{F}}_p\mathbf{F}_p^{-1}\mathbf{U}_e^{-1})_{skw}\tilde{\mathbf{R}}^T \\
&\approx \dot{\tilde{\mathbf{R}}}\tilde{\mathbf{R}}^T + \tilde{\mathbf{R}}(\dot{\mathbf{U}}_e(\mathbf{1}-\mathbf{U}_e))_{skw}\tilde{\mathbf{R}}^T + \tilde{\mathbf{R}}\mathbf{W}_p\tilde{\mathbf{R}}^T \quad , \quad \mathbf{W}_p := (\dot{\mathbf{F}}_p\mathbf{F}_p^{-1})_{skw} \equiv (\dot{\mathbf{U}}_p\mathbf{U}_p^{-1})_{skw} + \dot{\mathbf{R}}_p\mathbf{R}_p^T \\
&\approx \dot{\tilde{\mathbf{R}}}\tilde{\mathbf{R}}^T + \tilde{\mathbf{R}}\mathbf{W}_p\tilde{\mathbf{R}}^T
\end{aligned}$$

If $\mathbf{W}_p$ is identical to zero due to a corresponding $\mathbf{R}_p$-process (Gurtin & Anand, 2005a), then the Jaumann-spin $(\dot{\mathbf{F}}\mathbf{F}^{-1})_{skw}$ would arise for the spin $\dot{\tilde{\mathbf{R}}}\tilde{\mathbf{R}}^T$, with which the Cauchy stress tensor is rotated according to eq. (2.14)a. But $\mathbf{W}_p$ is not generally zero under the physical assumption (3.7), $\mathbf{R}_p \equiv \mathbf{1}$, for the description of initially isotropic materials without strong texture development. Thus, using $\mathbf{W}_p \equiv \mathbf{0}$, a special kind of deformation-induced anisotropy is described by the development of a plastic rotation $\mathbf{R}_p$ of the material with respect certain material directions (Mandel, 1974; Rice, 1975) due to $\mathbf{W}_p \equiv \mathbf{0}$, see the definition of $\mathbf{W}_p$ above.

at large plastic deformation (Bammann, 1984). But kinematic hardening is neglected in this section where the influence of the gradient-dependence of damage is investigated.

5.2 Gradient-dependent damage evolution equations

The responses of two gradient-dependent damage models are compared:

(i) the rate-dependent version (4.9)

$$\mathrm{W_c}\,\dot{s} \;=\; \sigma_{\mathrm{eq,eff}}\,\dot{p} \;+\; \mathrm{k}_2\,\Delta s \quad , \quad \sigma_{\mathrm{eq,eff}} := \frac{\sigma_{\mathrm{eq}}}{1-\mathrm{D}} \quad , \quad \mathrm{D}(s) = s^{\mathrm{r}} \tag{5.5}$$

and

(ii) the quasi-rate-independent form (4.10)

$$\mathrm{W_c}\,\dot{s} \;=\; \left(\sigma_{\mathrm{eq,eff}} + \mathrm{k}\,\Delta s\right)\dot{p} \tag{5.6}$$

The weak formulation of the partial differential equations (5.5, 6) can be formalised with the higher stress vector $\mathbf{b}_s$ according to (4.5) as

$$\int_v \left(\kappa_s(\dot{s}) - \tilde{y} - \mathbf{b}_s\cdot\nabla\right)\delta s\; dV = 0 \tag{5.7}$$

⇔

$$\int_v \left((\kappa_s(\dot{s}) - \tilde{y})\,\delta s - (\mathbf{b}_s\,\delta s)\cdot\nabla + \mathbf{b}_s\cdot(\nabla\delta s)\right) dV = 0 \tag{5.8}$$

with

(i) $\kappa_s(\dot{s}) \equiv \mathrm{W_c}\,\dot{s}$ and $\tilde{y} \equiv \sigma_{\mathrm{v,eff}}\,\dot{p}$ for rate-dependent damage (5.5) and

(ii) $\kappa_s(\dot{s}) \equiv \mathrm{W_c}\,\dfrac{\dot{s}}{\dot{p}}$ and $\tilde{y} \equiv \sigma_{\mathrm{v,eff}}$ in the quasi-rate-independent case (5.6)

integrating over the body volume in the initial (reference) placement. Application of Gauß's theorem yields

$$\int_v \left((\kappa_s(\dot{s}) - \tilde{y})\,\delta s + \mathbf{b}_s\cdot(\nabla\delta s)\right) dV = \int_{\partial v} \delta s\,\mathbf{b}_s\cdot\mathbf{n}\; dA \tag{5.9}$$

As boundary condition the higher stress $\mathbf{b}_s\cdot\mathbf{n}$ on the surface of a body is assumed to be zero.

The weak formulation (5.7) was implemented at the user-element interface (UEL) of ABAQUS/Standard (Sievert & Kiyak, 2005; compare Reusch, 2003; Hibbit et al., 2001).

As a viscoplastic flow rule, simply a power law with isotropic hardening is used

$$\mathbf{D}_p^R = \dot{p}\,\vec{\mathbf{D}}_p^R \quad , \quad \dot{p} = \dot{p}_0\left(\frac{\sigma_{\mathrm{eq,eff}}}{\mathrm{A} + \mathrm{B}\,p^m}\right)^n \quad , \quad \vec{\mathbf{D}}_p^R = \sqrt{\frac{3}{2}}\,\frac{\boldsymbol{\tau}^{R'}}{\left\|\boldsymbol{\tau}^{R'}\right\|} \tag{5.10}$$

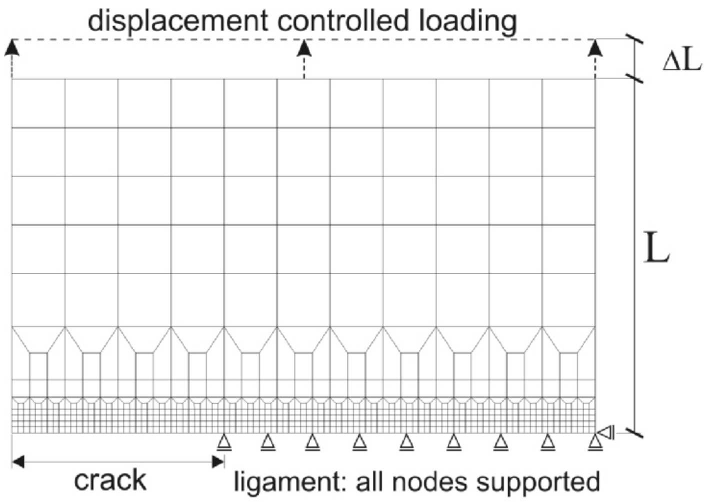
The following high strength material constants were chosen: n = 9, A = 650 MPa, B = 1700 MPa, m = 0.4, $\dot{p}_0 = 10^{-3}$ 1/s; $\mathrm{W_c}$ = 200 MPa, r = 12.

For viscoplastic stress-strain behaviour eq. (5.6) describes still a quasi-rate-independent damage evolution.

The gradient stiffness k_2 and k in the gradient-dependent damage evolution equation (5.5) and (5.6), respectively, have been determined by consideration of a shear-banding in a plane-strain layer, initialized by lateral geometrical imperfections, under quasi-static tensile loading (Sievert & Kiyak, 2005). The simulated shear-band widths converged upon mesh-refinement. The values of the material paramters k_2 = 0,05 MPa mm^2/s and k = 3 MPa mm^2 were chosen so that the simulated shear-band widths took reasonable sizes.

The pure local rate-dependent model has lead to much smaller shear band widths, which did not converge for the investigated finite element meshes up to about 50 elements over the entire layer width. Much more refined meshes are out of the engineering practice due to the needed computation time. Flatten (2008) showed analytically by stability considerations that an internal length due to the viscosity of a rate-dependent pure local model decreases continuously with increasing plastic strain-rate for a nonlinear strain-rate dependence of the stress. Thus, at increasing plastic strain-rate due to localisation the regularisation effect of such a model decreases, then the width of the simulated localisation zone decreases and the plastic strain-rate increases again. Flatten (2008) showed further that only for the special case of the linear strain-rate dependence of a pure local model the internal length due to the viscosity is totally independent of the plastic strain-rate, and thus, it gives a significant regularisation effect at the finite-element simulation of localisation (Sluys, 1992). But in the present investigation a nonlinear strain-rate dependence is considered throughout the work.

A thermomechanically loaded structure, e.g. a turbine blade, is loaded essentially strain-controlled by the constrained thermal strain due to the spatially inhomogeneous temperature distribution. This causes a mechanical strain. An in-service loading corresponds then to a strain hold-time period.



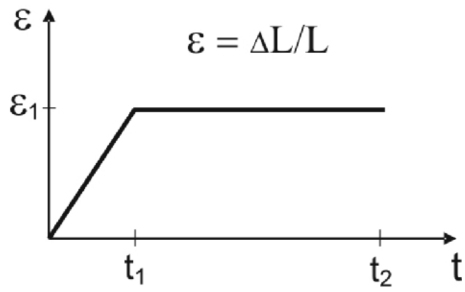


Figure 1. Loading of a crack by a global strain ε: **a** geometry, **b** time-function; crack depth: 3.6 mm, ligament length: 6.3 mm, L = 6 mm

When applying a more dangerous global tensile strain hold-time to a crack, Figure 1, in a viscoplastic material, the stresses are relaxing, Figure 2a,b, and the viscoplastic strain-rate reduces strongly, Figure 2c. But according to the rate-dependent damage evolution equation (5.5) the damage decreases, too, Figure 2d and Figure 3b, which is physically not meaningful if healing effects are not significant in the material.

Using the quasi-rate-independent damage model (5.6) the damage evolution is strongly reduced during the hold-time due to the relaxing stresses, but in this case the damage does not decrease, see Figure 2d and Figure 3d. This is due to the proportionality of the entire damage evolution equation (5.6) to the equivalent plastic strain-rate which reduces by orders of magnitudes at stress relaxation, Figure 2c, and thus the damage-rate reduces, too, but it is still positive according to the quasi-rate-independent damage model, Figure 2d. Of course, the Laplace-term in eq. (5.6) acts as a back-stress with respect to the damage evolution. But for a low equivalent effective stress, the equivalent plastic strain-rate is also low according to the flow rule (5.10)b, and thus, a formally possible negative damage-rate at low equivalent effective stress due to a negative Laplace term is negligible in the quasi-rate-independent damage model (5.6).

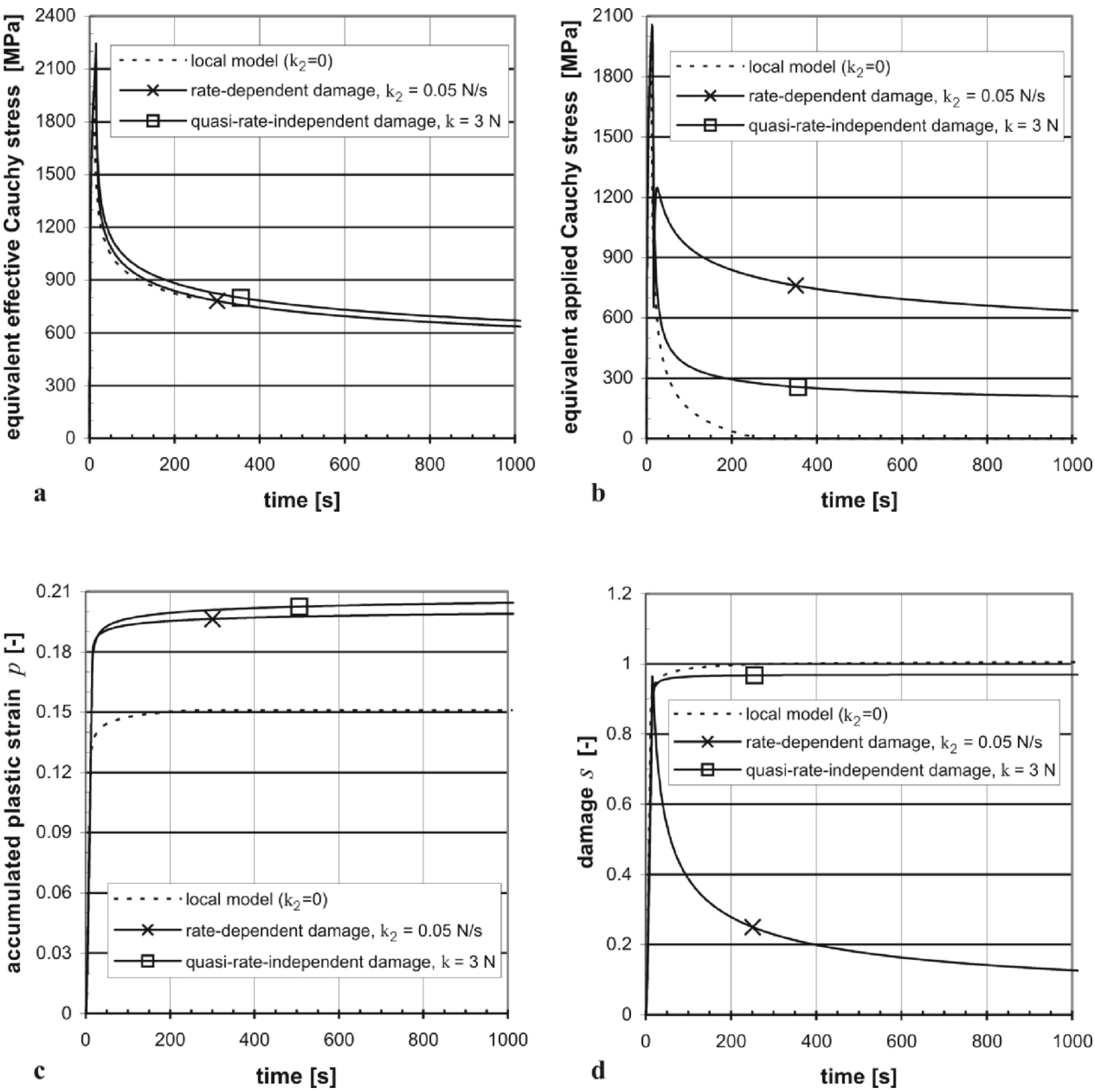


Figure 2. a Equivalent effective Cauchy stress $\sigma_{eq,eff}$ and **b** equivalent applied Cauchy stress σ_{eq} relaxations, as well as **c** development of accumulated viscoplastic strain and **d** evolution of the internal time s for damage at a crack tip during a global strain hold period (compare Figure 1) according to the local model and two gradient-dependent damage models, eqs. (5.5,6); the global strain hold begins (t_1) in all cases when the internal time *s* for damage is close to 1 for the first time (t_1 = 10 – 15 s, see **d**)

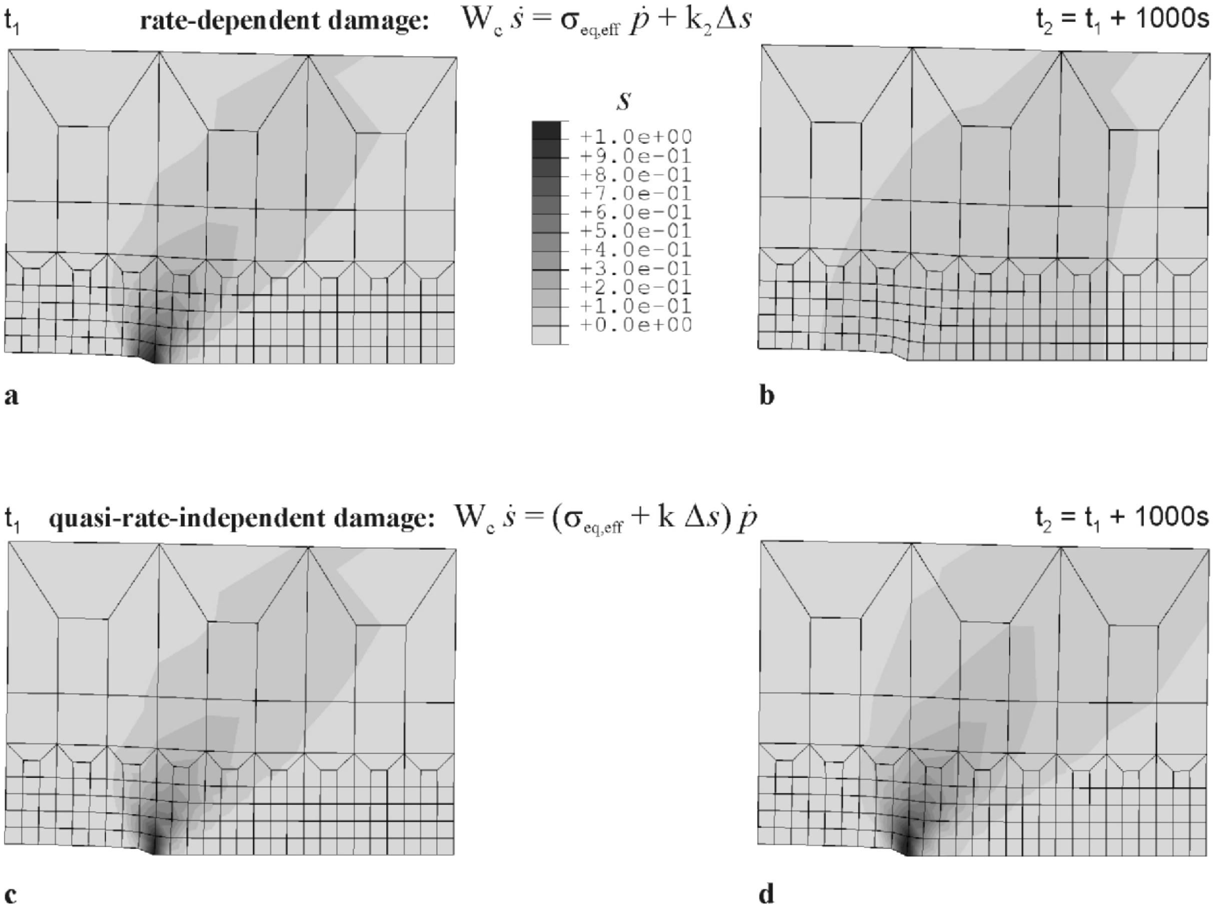


Figure 3. Internal time s for damage at a crack tip under plane strain according to two gradient-dependent damage models: **a**, **b** rate-dependent damage ($k_2 = 0.05$ N/s) and **c**, **d** quasi-rate-independent, i.e. fully plastic strain controlled, damage ($k = 3$ N); after monotonous tensile loading (**a**, **c**) and after the subsequent stress-relaxation hold-time period (**b**, **d**); compare Figure 1 for the loading conditions

6 Conclusion

A thermodynamically consistent finite deformation elasto-viscoplasticity theory of second grade has been presented that takes into account the spatial gradient of the elastic strain and of plastic internal strain tensors. For example, an internal strain tensor induced by viscoplastic straining was considered, by which energy due to hardening (latent energy) is stored also with its gradient. The evolution equations for these viscoplastic strains as partial differential equations of second order in space for these variables as well as the representation of the power of work at contact, required for the formulation of the additional boundary conditions, were derived via the dissipation inequality. In this way the well-known gradient-dependent viscoplastic flow rule of Zbib & Aifantis (1988) was thermodynamically founded and re-formulated in the presence of damage. Also a possible application of the present constitutive theory to polymers has been indicated.

In order to maintain the delocalizing effect of a gradient-dependent damage model for the same material even at higher strain rates, the damage evolution should be fully controlled by the plastic strain-rate. Therefore, a gradient-dependent damage model has been developed whose evolution equation is homogeneously of degree one in an equivalent plastic strain-rate, as common for hardening and softening relations controlled by plastic strain.

Finite-element simulations of a global strain hold-time period at a crack tip using the developed quasi-rate-independent gradient-enhanced damage model were compared with the simulations using a rate-dependent gradient-enhanced damage model. In a viscoplastic material the stresses are relaxing during a global strain hold period and thus the viscoplastic strain-rate is decreasing by orders of magnitude. Hence, in order to prevent a decrease of the simulated damage during the hold-time, if healing effects are negligible, the effect of the nonlocal term in a gradient-dependent evolution equation should also vanish when the plastic strain-rate reduces strongly. This is ensured by the proportionality of the entire evolution equation to the plastic strain-rate.

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Appendix A

Notation

A compact notation is used in this work with vectors and tensors denoted by boldface letters. The representation of these tensors of order one to four is with respect to a positively oriented orthonormal basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ in a three-dimensional Euclidean space

$$\mathbf{a} \equiv \mathrm{a}_i\, \mathbf{e}_i \quad , \quad \mathbf{B} \equiv \mathrm{B}_{ij}\, \mathbf{e}_i \otimes \mathbf{e}_j \quad , \quad \mathbf{C}_{ijk} \equiv \mathrm{C}_{ijk}\, \mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \quad , \quad \mathbf{D} \equiv \mathrm{D}_{ijkl}\, \mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l \tag{A.1}$$

with the dyadic product $\otimes$ and summation over all repeated indices. $\mathbf{1} := \delta_{ij}\, \mathbf{e}_i \otimes \mathbf{e}_j$ is the second order unity tensor with the Kronecker symbol δ_{ij}. The transpose of a second order tensor $\mathbf{B}$ is denoted by $\mathbf{B}^{\mathrm{T}} \equiv \mathrm{B}_{ij}\, \mathbf{e}_j \otimes \mathbf{e}_i$. The symmetric part of $\mathbf{B}$ is defined by $\mathbf{B}_{\mathrm{s}} := \frac{1}{2}\left(\mathbf{B}+\mathbf{B}^{\mathrm{T}}\right)$ and the skew-symmetric part as $\mathbf{B}_{\mathrm{skw}} := \frac{1}{2}\left(\mathbf{B}-\mathbf{B}^{\mathrm{T}}\right)$.

The inverse $\mathbf{A}^{-1}$ of a the linear transformation $\mathbf{A}$ is defined by

$$\mathbf{y} = \mathbf{A}\cdot\mathbf{x} \quad , \quad \mathbf{A}^{-1}\cdot\mathbf{y} := \mathbf{x} \tag{A.2}$$

The linear mapping of second order tensors connected in series, resulting in a new second order tensor, is denoted without a product symbol: $\mathbf{C} = \mathbf{A}\,\mathbf{B}$. Scalar products between tensors are denoted by dot marks with as many dots as couples of base vectors, directly at the left and right hand side next to the scalar product, shall be contracted successively by a simple vector scalar product, for example

$$\begin{aligned} &\mathbf{a}\cdot\mathbf{B} := \mathrm{a}_i\, \mathrm{B}_{ij}\, \mathbf{e}_j \quad , \quad \mathbf{A}\cdot\cdot\mathbf{B} := \mathrm{A}_{ij}\, \mathrm{B}_{ji} \equiv \mathbf{B}\cdot\cdot\mathbf{A} \quad , \quad \mathbf{A}:\mathbf{B} := \mathbf{A}\cdot\cdot\mathbf{B}^{\mathrm{T}} \equiv \mathrm{A}_{ij}\, \mathrm{B}_{ij} \\ &\mathbf{B}\cdot\cdot\mathbf{C} := \mathrm{B}_{ij}\, \mathrm{C}_{jik}\, \mathbf{e}_k \quad , \quad \mathbf{D}\cdot\cdot\mathbf{C} := \mathrm{D}_{ijkl}\, \mathrm{C}_{lkm}\, \mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_m \\ &\mathbf{D}\cdot\mathbf{B} := \mathrm{D}_{ijkl}\, \mathrm{B}_{lm}\, \mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_m \end{aligned} \tag{A.3}$$

The identity $\mathbf{A}\cdot\cdot(\mathbf{B}\cdot\mathbf{C}) \equiv (\mathbf{A}\cdot\mathbf{B})\cdot\cdot\mathbf{C}$ is extensively used.

The Euclidean norm of a tensor $\mathbf{A}$ is defined by

$$\|\mathbf{A}\| := (\mathbf{A}\cdot\cdot\mathbf{A}^{\mathrm{T}})^{1/2} \tag{A.4}$$

The fourth-order transposition tensor $\mathbf{1}_{\mathrm{T}}$ is defined by the linear mapping

$$\mathbf{1}_{\mathrm{T}}\cdot\cdot\mathbf{A} := \mathbf{A}^{\mathrm{T}} \quad \Leftrightarrow \quad \mathbf{1}_{\mathrm{T}} \equiv \mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_i \otimes \mathbf{e}_j \tag{A.5}$$

The nabla operator $\nabla := \dfrac{\partial}{\partial \mathrm{X}_i}\, \mathbf{e}_i$ is used to compute the gradient or divergence of tensors. The symbol $:=$ means equality by definition and the symbol $\equiv$ means the identification of functions. Other symbols are defined in the text at their first appearance. For further tensor algebra and analysis, see, e.g., Trostel (1993, 1997).

Appendix B

Representation of the stresses depending on gradients only of scalar elastic quantities

By the volumetric elastic stretch

$$\det \mathbf{U}_e =: J_e \equiv (\det \mathbf{C}_e)^{\frac{1}{2}} \tag{B.1}$$

one can define an isochoric elastic stretch tensor as counterpart (Flory, 1961)

$$\bar{\mathbf{U}}_e := J_e^{-\frac{1}{3}}\,\mathbf{U}_e \qquad \Rightarrow \qquad \det\bar{\mathbf{U}}_e \equiv 1 \tag{B.2)a}$$

with

$$\left\|\bar{\mathbf{U}}_e\right\|^2 = \bar{\mathbf{U}}_e\cdot\cdot\,\bar{\mathbf{U}}_e = \mathbf{1}\cdot\cdot\,\bar{\mathbf{C}}_e =: \operatorname{tr}\bar{\mathbf{C}}_e =: \bar{\mathrm{I}}_e \qquad , \qquad \bar{\mathbf{C}}_e := \bar{\mathbf{U}}_e^2 \equiv J_e^{-\frac{2}{3}}\,\mathbf{C}_e \tag{B.2)b,c}$$

Here, energy storage with the gradient of elastic strain shall be considered which depends primarily only on the gradients of the quantities (B.1,2)

$$\rho\psi = \tilde{\psi}\left(\mathbf{C}_e, \nabla\bar{\mathrm{I}}_e, \nabla J_e, \boldsymbol{\alpha}, \boldsymbol{\alpha}\otimes\nabla\right) \tag{B.3}$$

The time derivative of this strain energy function is then

$$\begin{aligned}\rho\dot{\psi} &= \dot{\mathbf{C}}_e\cdot\cdot\frac{\partial\tilde{\psi}}{\partial\mathbf{C}_e} + \left(\dot{\bar{\mathrm{I}}}_e\frac{\partial\tilde{\psi}}{\partial\nabla\bar{\mathrm{I}}_e} + \dot{J}_e\frac{\partial\tilde{\psi}}{\partial\nabla J_e}\right)\cdot\nabla - \dot{\bar{\mathrm{I}}}_e\left(\frac{\partial\tilde{\psi}}{\partial\nabla\bar{\mathrm{I}}_e}\cdot\nabla\right) - \dot{J}_e\left(\frac{\partial\tilde{\psi}}{\partial\nabla J_e}\cdot\nabla\right)\\ &\quad + \left(\dot{\boldsymbol{\alpha}}\cdot\frac{\partial\tilde{\psi}}{\partial\boldsymbol{\alpha}\otimes\nabla}\right)\cdot\nabla + \dot{\boldsymbol{\alpha}}\cdot\left(\frac{\partial\tilde{\psi}}{\partial\boldsymbol{\alpha}} - \frac{\partial\tilde{\psi}}{\partial\boldsymbol{\alpha}\otimes\nabla}\cdot\nabla\right)\end{aligned} \tag{B.4}$$

The time derivatives of the quantities $\bar{\mathrm{I}}_e$ and J_e are

$$\dot{J}_e \equiv \dot{\mathbf{C}}_e\cdot\cdot\frac{\mathrm{d}J_e}{\mathrm{d}\mathbf{C}_e} = \dot{\mathbf{C}}_e\cdot\cdot\mathbf{C}_e^{-1}\,\tfrac{1}{2}J_e \tag{B.5}$$

and

$$\begin{aligned}\dot{\bar{\mathrm{I}}}_e &= \mathbf{1}\cdot\cdot\left(J_e^{-\frac{2}{3}}\,\mathbf{C}_e\right)^{\boldsymbol{\cdot}} = J_e^{-\frac{2}{3}}\,\mathbf{1}\cdot\cdot\,\dot{\mathbf{C}}_e - \tfrac{2}{3}J_e^{-\frac{2}{3}}J_e^{-1}\,\mathbf{1}\cdot\cdot\,\mathbf{C}_e\,\tfrac{1}{2}J_e\,\mathbf{C}_e^{-1}\cdot\cdot\,\dot{\mathbf{C}}_e\\ &= \dot{\mathbf{C}}_e\cdot\cdot\left(\mathbf{C}_e^{-1}\cdot\bar{\mathbf{C}}_e'\right) \qquad , \qquad \bar{\mathbf{C}}_e' := \bar{\mathbf{C}}_e - \tfrac{1}{3}\operatorname{tr}\bar{\mathbf{C}}_e\,\mathbf{1}\end{aligned} \tag{B.6}$$

By inserting eqs. (B.5,6) into (B.4)

$$\begin{aligned}\rho\dot{\psi} &= \left[\dot{\mathbf{C}}_e\cdot\cdot\left(\mathbf{C}_e^{-1}\cdot\left(\bar{\mathbf{C}}_e'\otimes\frac{\partial\tilde{\psi}}{\partial\nabla\bar{\mathrm{I}}_e} + \tfrac{1}{2}J_e\,\mathbf{1}\otimes\frac{\partial\tilde{\psi}}{\partial\nabla J_e}\right)\right)\right]\cdot\nabla\\ &\quad + \dot{\mathbf{C}}_e\cdot\cdot\left[\frac{\partial\tilde{\psi}}{\partial\mathbf{C}_e} - \mathbf{C}_e^{-1}\cdot\left(\bar{\mathbf{C}}_e'\left(\frac{\partial\tilde{\psi}}{\partial\nabla\bar{\mathrm{I}}_e}\cdot\nabla\right) - \tfrac{1}{2}J_e\,\mathbf{1}\left(\frac{\partial\tilde{\psi}}{\partial\nabla J_e}\cdot\nabla\right)\right)\right]\\ &\quad + \left(\dot{\boldsymbol{\alpha}}\cdot\frac{\partial\tilde{\psi}}{\partial\boldsymbol{\alpha}\otimes\nabla}\right)\cdot\nabla + \dot{\boldsymbol{\alpha}}\cdot\left(\frac{\partial\tilde{\psi}}{\partial\boldsymbol{\alpha}} - \frac{\partial\tilde{\psi}}{\partial\boldsymbol{\alpha}\otimes\nabla}\cdot\nabla\right)\end{aligned} \tag{B.7}$$

and using eq. (2.6)

$$\begin{aligned}\rho\dot{\psi} &= \left[\left(\dot{\mathbf{U}}_e\mathbf{U}_e^{-1}\right)_s\cdot\cdot\left(\bar{\mathbf{C}}_e'\otimes 2\frac{\partial\tilde{\psi}}{\partial\nabla\bar{\mathrm{I}}_e} + J_e\,\mathbf{1}\otimes\frac{\partial\tilde{\psi}}{\partial\nabla J_e}\right)\right]\cdot\nabla\\ &\quad + \left(\dot{\mathbf{U}}_e\mathbf{U}_e^{-1}\right)_s\cdot\cdot\left(\mathbf{U}_e\,2\frac{\partial\tilde{\psi}}{\partial\mathbf{C}_e}\,\mathbf{U}_e - \bar{\mathbf{C}}_e'\left(2\frac{\partial\tilde{\psi}}{\partial\nabla\bar{\mathrm{I}}_e}\cdot\nabla\right) - J_e\,\mathbf{1}\left(\frac{\partial\tilde{\psi}}{\partial\nabla J_e}\cdot\nabla\right)\right)\\ &\quad + \left(\dot{\boldsymbol{\alpha}}\cdot\frac{\partial\tilde{\psi}}{\partial\boldsymbol{\alpha}\otimes\nabla}\right)\cdot\nabla + \dot{\boldsymbol{\alpha}}\cdot\left(\frac{\partial\tilde{\psi}}{\partial\boldsymbol{\alpha}} - \frac{\partial\tilde{\psi}}{\partial\boldsymbol{\alpha}\otimes\nabla}\cdot\nabla\right)\end{aligned} \tag{B.8}$$

the following re-definitions can be made for the observer-invariant Kirchhoff stress tensors working on the elastic strain-rate of the current configuration, compare eq. (2.9)

$$\mathbf{T}^R := \bar{\mathbf{C}}'_e \otimes 2\frac{\partial\tilde{\psi}}{\partial\nabla\bar{\mathrm{I}}_e} + J_e\,\mathbf{1}\otimes\frac{\partial\tilde{\psi}}{\partial\nabla J_e} \tag{B.9}$$

$$\boldsymbol{\tau}^R := \mathbf{U}_e 2\frac{\partial\tilde{\psi}}{\partial\mathbf{C}_e}\mathbf{U}_e - \bar{\mathbf{C}}'_e\left(2\frac{\partial\tilde{\psi}}{\partial\nabla\bar{\mathrm{I}}_e}\cdot\nabla\right) - J_e\,\mathbf{1}\left(\frac{\partial\tilde{\psi}}{\partial\nabla J_e}\cdot\nabla\right) \tag{B.10}$$

The Mandel stress (2.15) reads then as

$$\mathbf{M} := \mathbf{U}_e\boldsymbol{\tau}^R\mathbf{U}_e^{-1} \equiv 2\mathbf{C}_e\frac{\partial\tilde{\psi}}{\partial\mathbf{C}_e} - \bar{\mathbf{C}}'_e\left(2\frac{\partial\tilde{\psi}}{\partial\nabla\bar{\mathrm{I}}_e}\cdot\nabla\right) - J_e\,\mathbf{1}\left(\frac{\partial\tilde{\psi}}{\partial\nabla J_e}\cdot\nabla\right) \tag{B.11}$$

For the consideration of the strain energy as a certain function of the isochoric Cauchy-Green tensor $\bar{\mathbf{C}}_e$ and the volumetric stretch J_e instead of $\mathbf{C}_e$ with respect to the first terms on the right hand-sides in eqs. (B.10) and (B.11), see Simo & Hughes (1998, pp. 358).

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