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The fundamental role of nonlocal and local balance laws of material forces in finite elastoplasticity and damage mechanics

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Abstract

In this paper the fundamental role of independent balance laws of material forces acting on dislocations and microdefects is shown. They enable a thermodynamically consistent formulation of dissipative deformation processes of continua with dislocation motion and defect evolution in the material space on meso- and microlevel.

The balance laws of material forces together with the classical balance laws of physical forces and couples, first and second laws of thermodynamics for physical and material space and general constitutive equations are the basis to develop a thermodynamically consistent framework of nonlocal finite elastoplasticity and brittle and ductile damage.

It is shown that a weakly-nonlocal formulation of the balance laws of material forces leads to gradient theories, where local theories are obtained, if all gradient contributions are assumed to be small. In this case the local balance laws of material forces together with the constitutive equations represent evolution laws of the material forces. In the classical approach of internal variables they are assumed from the outset with the result that there is a large number of different propositions in the literature.

The well-known splitting test of a circular cylinder of concrete is simulated numerically, where the process of deformation in the physical space and defect and plastic evolution in the material space is represented.

Keywords: Brittle damage; Ductile damage; Gradient damage; Gradient elastoplasticity; Material forces; Configurational forces; Dissipative processes

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1. Introduction

Motion and deformation of continua in the physical space are well defined within the concept of classical continuum mechanics and, if temperature changes are taken into account, within classical continuum thermodynamics. They are based on the postulates of physical linear and angular momentum and first and second law of thermodynamics supplemented by appropriate constitutive equations subject to objectivity requirements (Truesdell and Noll, 1965). In general, along with the deformation of the material body in the physical space a change of the internal material structure can occur accompanied by degradation of material properties. These changes are caused by physical mechanisms in the material space on macro-, meso-, and microlevel, respectively, where microcracks, microvoids and dislocations are observed in brittle and ductile material, respectively.

An appropriate description of nucleation and evolution of microdefects and their coupling with the deformation of the body in the physical space is not at all an easy task. Most concepts proposed so far in the literature of elastoplasticity and damage are internal variable approaches (see e.g. Kachanov, 1986; Chaboche, 1988; Hansen and Schreyer, 1994; Krajcinovic, 1996; Houlsby and Puzrin, 2000). Internal variable approaches are based on classical continuum mechanics to describe the macrodeformation, while the nucleation and evolution of microdefects are characterized by internal variables, for which evolution laws are postulated. Essential drawbacks of these theories are:

- Internal variable approaches are local theories, which are not able to describe appropriately localization phenomena (e.g. Bažant, 1991) leading to a pathological mesh-dependency of corresponding FE-solutions (see e.g. Miehe, 1998; Schieck et al., 1999);
- Local theories are not able to simulate length scale dependent problems (see e.g. Bažant and Ožbolt, 1990; Bažant and Planas, 1998);
- There is no recipe, how to chose evolution laws. Therefore, there are quite different propositions in the literature.

To overcome the numerical difficulties associated with the analysis of localization phenomena applying local theories integral and gradient enhancements were proposed in the literature (e.g. Aifantis, 1984; Bažant and Pijaudier-Cabot, 1988; de Borst and Mühlhaus, 1992; de Borst et al., 1995; de Borst, 2001), where the gradient enhancements can be obtained from integral enhancements by Taylor expansion restricting to the first term of the series. Gradient theories are weakly-nonlocal, but with the advantage that they are better accessible to numerical applications than integral enhanced theories. Fully nonlocal theories can be established also by taking into account the manifold structure of the material space with torsion and curvature (see e.g. Shizawa and Zbib, 1999; Cleja-Tigoiu, 2002a,b; Rakotomanana, 2004; Clayton et al., in press).

While the question of locality or nonlocality of the model is essential for the numerical analysis of localization phenomena as shearbands and damage concentrations, it does not explain the large number of proposed theories in finite elastoplasticity and damage mechanics and many controversial discussions in the literature on these fields. The crucial point and reason for this is the fact that in general to describe the dissipative process of defect evolution on meso- and mirolevel there are less equations than unknowns and therefore the missing equations are freely assumed as in the case of evolution laws.

Since Leibfried (1949), Peach and Koehler (1950) and Eshelby (1951) it is known that there are forces acting on microdefects as microcracks, voids and dislocations, and these forces are non-standard and called "material forces" and "configurational forces", respectively, contrary to the Newtonian "physical forces" acting on masses in the physical space. The material forces have to satisfy their own dynamical balance laws, which are independent of the balance laws of physical forces, coupled only by constitutive equations.

The fundamental role of the material force balances and their consequences for the formulation of finite elastoplasticity and brittle and ductile damage is subject of this paper.

Models of finite elastoplasticity based on an additional independent balance law of material forces on dislocations were presented for non-dissipative equilibrium forces in Naghdi and Srinivasa (1993a,b), Stumpf and Le (1993) and Le and Stumpf (1996a). The latter theory is generalized in Le and Stumpf (1996b) for rate-dependent gradient elastoplasticity taking into account besides the non-dissipative equilibrium forces also the dissipative driving forces on dislocations. In Le and Stumpf (1996c) it is shown that within this concept the plastic deformation, $\mathbf{F}^{\mathrm{p}} = \mathbf{R}^{\mathrm{p}}\mathbf{U}^{\mathrm{p}}$, and the plastic rotation $\mathbf{R}^{\mathrm{p}}$ can be determined uniquely (up to rigid body rotation). While these theories are based on weakly-nonlocal balance laws of material forces, Cermelli et al. (2001) presented a closed concept of finite elastoplasticity postulating a local balance law of the material forces on dislocations. This theory allows to determine uniquely the evolution of the plastic deformation.

A weakly-nonlocal model of rate-independent crystal plasticity is presented in Gurtin (2000) taking into account the dependency on plastic strain gradients. The theory is based on microforce balances in addition to the classical physical force balance. As a consequence of the second law of thermodynamics the internal microforces are given in terms of energetic and dissipative parts, where the energetic parts are derived from the free energy.

In damage mechanics Frémond and Nedjar (1996) presented a virtual work principle for isotropic brittle damage leading to the classical force balance and an additional weakly-nonlocal balance of a scalar-valued material force power-conjugate to the scalar-valued damage parameter. A gradient theory of anisotropic brittle damage with an additional balance law of material forces acting on microdefects is derived in Stumpf and Hackl (2003).

Fully nonlocal damage theories with additional material force balances are subject of the papers Stumpf and Saczuk (2000), Saczuk et al. (2001, 2003). These theories are based on the manifold structure of the material space, where the gradient operator is replaced by the so-called connection, which depends on torsion (dislocations) and curvature (disclinations) of the manifold (see also Rakotomanana, 2004). In Makowski and Stumpf (2001) the structure of the material space is modeled by a finite set of directors, where for the power-conjugate material forces independent balance laws are introduced. Contrary to the weakly-nonlocal (gradient-type) models, the fully nonlocal theories are so far not accessible to numerical applications.

The paper is organized as follows. In Section 2 independent kinematical variables are introduced to describe the position and motion of material particles in the physical space and the evolution of microcracks, microvoids and dislocations on meso- and microlevel in the material space. Power-conjugate physical and material forces are defined and independent integral balance laws for physical forces and couples and material forces are postulated, from which their local forms can be derived. Corresponding to these balance laws the principle of virtual power for physical and material space is given. Next the first and second law of thermodynamics are formulated for physical and material space in integral form and their local forms are derived.

In Section 3 general constitutive equations for the free energy and for physical and material stresses are assumed as function of the physical deformation gradient and its rate and the material kinematical variables, their gradients and rates. The thermodynamically admissible form of the constitutive equations is determined showing that all forces and stresses, respectively, consist of a non-dissipative part, which can be derived from the free energy potential, and a dissipative part representing the driving forces on defects and dislocations on meso- and microlevel. They have to satisfy the dissipation inequality. It is shown that under certain symmetry conditions a dissipation pseudo-potential exists allowing to express the constitutive equations by two potentials, the free energy and the dissipation pseudo-potential. Finally in Section 3 the governing equations for the analysis of isothermal, dissipative deformation processes with defect and plastic evolution are presented.

In Section 4 simplified weakly-nonlocal models of damage and finite elastoplasticity are investigated: an isotropic gradient model of brittle and ductile damage and a model of finite elastoplasticity with gradient isotropic hardening. In Section 5 numerical results are presented for the splitting test of a concrete cylinder applying the isotropic gradient damage model for brittle and ductile material behavior.

2. Kinematics and general laws in physical and material space

2.1. Kinematical variables in the physical space

In classical Newtonian mechanics the motion of material points for continuous media can be defined by a vector-value function, the actual position vector $\mathbf{x}(\mathbf{X},t)$ or the corresponding displacement vector $\mathbf{u}(\mathbf{X},t)$,

$$\mathbf{x} = \mathbf{x}(\mathbf{X},t) = \mathbf{X} + \mathbf{u}(\mathbf{X},t), \tag{2.1}$$

where $\mathbf{X}$ is the position vector in the undeformed and homogeneous reference configuration, and t is the time parameter.

Once the mapping (2.1) is given, all kinematical variables on the macrolevel are specified, in particular the velocity

$$\mathbf{v}(\mathbf{X},t) = \dot{\mathbf{x}}(\mathbf{X},t), \tag{2.2}$$

where a dot denotes the material time derivative, the deformation gradient

$$\mathbf{F}(\mathbf{X},t) = \nabla\mathbf{x}(\mathbf{X},t) = \mathbf{1} + \nabla\mathbf{u}(\mathbf{X},t), \tag{2.3}$$

the Cauchy–Green deformation tensor $\mathbf{C}(\mathbf{X},t)$ and the Green strain tensor $\mathbf{E}(\mathbf{X},t)$,

$$\mathbf{C} = \mathbf{F}^{\mathrm{T}}\mathbf{F}, \quad \mathbf{E} = \frac{1}{2}(\mathbf{F}^{\mathrm{T}}\mathbf{F} - \mathbf{1}), \tag{2.4}$$

where $\mathbf{1}$ is the identity tensor.

In this paper we apply a Lagrangian formulation of all equations, it means that all fields are referred to the undeformed and homogeneous reference configuration. The corresponding Euler formulation can then be obtained easily by push-forward operation of all quantities to the actual configuration (see e.g. Stumpf and Hoppe, 1997).

Material points of continuous media have three degrees of freedom. Therefore, (2.1) defines for continuous media the motion of material points in the physical space uniquely. On the other side, granular media have six degrees of freedom, three translational and three rotational ones. While the translational motion is described by (2.1), the rotational part of the motion can be defined by a rotation tensor in the case of finite rotations and by a rotation vector in the case of small rotations (Makowski et al., 2004). In the present paper we shall restrict our considerations to dissipative deformation processes of continuous media.

2.2. Kinematical variables in the material space

While for continuous media the motion in the physical space, deformation and strains are defined by (2.1)–(2.4), inside the material space the nucleation and evolution of microcracks, microvoids, microshear bands and dislocations are observed on meso- and microlevel, respectively, leading to material degradation and damage as well as to plastic material changes. Since these physical phenomena are quite different, we introduce for their description two independent kinematical tensor functions, $\mathbf{F}^{\mathrm{d}}(\mathbf{X},t)$ and $\mathbf{F}^{\mathrm{p}}(\mathbf{X},t)$, associated with damage, $(\bullet)^{\mathrm{d}}$, and plasticity $(\bullet)^{\mathrm{p}}$.

In the simplest case of isotropic damage $\mathbf{F}^{\mathrm{d}}(\mathbf{X},t)$ reduces to $\mathbf{F}^{\mathrm{d}}(\mathbf{X},t)=D(\mathbf{X},t)\mathbf{1}$, where $\mathbf{1}$ is the identity tensor and $D(\mathbf{X},t)$ a scalar-valued function within the range $[0,1]$, $D=0$ corresponding to the undamaged state and $D=1$ to the fully damaged state. As physical interpretation the scalar-valued damage function D may represent the amount of microcracks and/or microvoids in a representative volume element. To take into account that microcracks have an orientation an anisotropic damage description can be needed. In this case $\mathbf{F}^{\mathrm{d}}(\mathbf{X},t)$ may be considered as a symmetric tensor function referred to the homogeneous reference configuration (Stumpf and Hackl, 2003).

To describe the plastic deformation inside the material space, we chose the so-called plastic deformation gradient $\mathbf{F}^{\mathrm{p}}(\mathbf{X},t)$, which is a locally defined linear map and not a gradient of the type (2.3), because there exists no associated displacement field. Applying the polar decomposition theorem, $\mathbf{F}^{\mathrm{p}}=\mathbf{R}^{\mathrm{p}}\mathbf{U}^{\mathrm{p}}$, with the Lagrangian plastic stretch $\mathbf{U}^{\mathrm{p}}$ and the plastic rotation $\mathbf{R}^{\mathrm{p}}$, it follows that $\mathbf{F}^{\mathrm{p}}$ has nine independent components, six due to the plastic stretch $\mathbf{U}^{\mathrm{p}}$ and three due to the plastic rotation $\mathbf{R}^{\mathrm{p}}$. To analyze engineering structures at finite elastic–plastic strains a model can be constructed depending on the plastic stretch $\mathbf{U}^{\mathrm{p}}$ only and not on the plastic rotation $\mathbf{R}^{\mathrm{p}}$ (Schieck and Stumpf, 1995; Miehe, 1998; Schieck et al., 1999). For small deformations this corresponds to a formulation in linear plastic strains with six independent components. To take into account also the development of plastic anisotropies and strain hardening, both effects may depend on $\mathbf{F}^{\mathrm{p}}(\mathbf{X},t)$. In this case they are not independent variables.

In this paper an additional independent kinematical variable of the material space is introduced, $\xi^{\mathrm{p}}(\mathbf{X},t)$, assumed here as n-dimensional vector representing e.g. hardening parameters. To follow the numerically-oriented literature of gradient enhanced elastoplasticity and damage (see e.g. de Borst et al., 1993; Sluys et al., 1993; Nedjar, 2001) we choose a vector and not a tensor representation of the hardening parameters (for crystal plasticity see also Gurtin, 2000).

We collect the independent kinematical material variables in the ordered set

$$\boldsymbol{\varepsilon}=\left\{\mathbf{F}^{\mathrm{d}}(\mathbf{X},t),\mathbf{F}^{\mathrm{p}}(\mathbf{X},t),\xi^{\mathrm{p}}(\mathbf{X},t)\right\}, \tag{2.5}$$

with the ordered set of material space gradients $\nabla\boldsymbol{\varepsilon}$,

$$\nabla\boldsymbol{\varepsilon}=\left\{\nabla\mathbf{F}^{\mathrm{d}}(\mathbf{X},t),\nabla\mathbf{F}^{\mathrm{p}}(\mathbf{X},t),\nabla\xi^{\mathrm{p}}(\mathbf{X},t)\right\}, \tag{2.6}$$

and the material time changes of (2.5),

$$\dot{\boldsymbol{\varepsilon}}=\left\{\dot{\mathbf{F}}^{\mathrm{d}}(\mathbf{X},t),\dot{\mathbf{F}}^{\mathrm{p}}(\mathbf{X},t),\dot{\xi}^{\mathrm{p}}(\mathbf{X},t)\right\}, \tag{2.7}$$

where ∇ denotes the gradient with respect to the homogeneous and undeformed reference configuration. It should be pointed out that with the gradients (2.6) three different length scales are introduced, one associated with damage localization, one with plastic localization as shearband formation and one with hardening concentration.

2.3. Physical and material forces and stresses

Power-conjugate to the physical deformation gradient $\mathbf{F}$ is the classical first Piola–Kirchhoff stress tensor $\mathbf{T}$, and power-conjugate to the set of kinematical material variables (2.5) is the ordered set of material forces

$$\boldsymbol{\sigma}=\left\{\mathbf{T}^{\mathrm{d}}(\mathbf{X},t),\mathbf{T}^{\mathrm{p}}(\mathbf{X},t),\mathbf{t}^{\mathrm{p}}(\mathbf{X},t)\right\}, \tag{2.8}$$

and power-conjugate to (2.6) is the ordered set of material stresses

$$\boldsymbol{\Sigma}=\left\{\mathsf{H}^{\mathrm{d}}(\mathbf{X},t),\mathsf{H}^{\mathrm{p}}(\mathbf{X},t),\mathbf{H}^{\mathrm{p}}(\mathbf{X},t)\right\}, \tag{2.9}$$

such that the stress power in physical and material space can be written as

$$\boldsymbol{\sigma} = \mathbf{T} \bullet \dot{\mathbf{F}} + \boldsymbol{\sigma} \bullet \dot{\boldsymbol{\varepsilon}} + \boldsymbol{\Sigma} \bullet \nabla \dot{\boldsymbol{\varepsilon}}, \tag{2.10}$$

derived in Section 2.5 as result of the weak form of the physical and material force balances.

2.4. Integral and local balance laws of physical and material forces

For the purpose of this paper, the material body under consideration may be identified with a region B in the physical space, which the body occupies in a fixed reference configuration. The motion of the body is then described by the mapping (2.1) and (2.2). We assume furthermore that the referential mass density $\rho_0(\mathbf{X})$ is independent of time so that the balance law of mass conservation is satisfied identically. Then, the classical integral balance laws of physical linear and angular momenta are defined as

$$\int_{\partial P} \mathbf{T}\mathbf{n}\,\mathrm{d}a + \int_P \mathbf{b}\,\mathrm{d}v = \frac{\mathrm{d}}{\mathrm{d}t}\int_P \mathbf{p}\,\mathrm{d}v, \tag{2.11}$$

$$\int_{\partial P} \mathbf{x} \times \mathbf{T}\mathbf{n}\,\mathrm{d}a + \int_P \mathbf{x} \times \mathbf{b}\,\mathrm{d}v = \frac{\mathrm{d}}{\mathrm{d}t}\int_P \mathbf{x} \times \mathbf{p}\,\mathrm{d}v \tag{2.12}$$

with the denotations:

$\mathbf{T}(\mathbf{X}, t)$: physical first Piola–Kirchhoff stress tensor,
$\mathbf{b}(\mathbf{X}, t)$: external physical body force,
$\mathbf{p}(\mathbf{X}, t)$: physical momentum density.

Here $\mathbf{n}(\mathbf{X})$ is the outward unit normal vector to the boundary ∂P of a subdomain $P \subset B$ occupied by any part of the body in the reference configuration.

We postulate that the material forces on meso- and microlevel have to satisfy their own weakly-nonlocal integral balance laws. Introducing a set $\boldsymbol{\beta}$ of external forces breaking e.g. internal material bonds,

$$\boldsymbol{\beta} = \left\{\mathbf{G}^{\mathrm{d}}(\mathbf{X}, t), \mathbf{G}^{\mathrm{p}}(\mathbf{X}, t), \mathbf{g}^{\mathrm{p}}(\mathbf{X}, t)\right\}, \tag{2.13}$$

and a set $\boldsymbol{\pi}$ of material momenta of dynamically evolving microdefects, dislocations and hardening phenomena,

$$\boldsymbol{\pi} = \left\{\mathbf{P}^{\mathrm{d}}(\mathbf{X}, t), \mathbf{P}^{\mathrm{p}}(\mathbf{X}, t), \mathbf{p}^{\mathrm{p}}(\mathbf{X}, t)\right\}, \tag{2.14}$$

then the balance laws of material forces on meso- and microlevel are postulated as

$$\int_{\partial P} \boldsymbol{\Sigma}\mathbf{n}\,\mathrm{d}a + \int_P (-\boldsymbol{\sigma} + \boldsymbol{\beta})\,\mathrm{d}v = \frac{\mathrm{d}}{\mathrm{d}t}\int_P \boldsymbol{\pi}\,\mathrm{d}v \tag{2.15}$$

representing with (2.8), (2.9), (2.13) and (2.14) three independent balance laws of material forces. In the formulation of the material balance laws it was taken into account that although defects have no mass, they have inertia resulting from the interactions of moving defects with the surrounding material (cf. the classical studies on dislocations, e.g. Nabarro, 1987 or Hirth and Lothe, 1982). The inertia effects due to high speed motion of dislocations as well as dynamic evolution of microvoids and other defects are account for in the balance law (2.15) through the material momentum density of the general form (2.14). For experimental data of crack propagation in rocks with small crack tip process zone of microcracks the reader may refer to Bertram and Kalthoff (2003).

Under the usual regularity requirements the local balance laws of physical linear and angular momenta can be derived from (2.11) and (2.12) yielding for every subbody $P \subset B$ the local balances of physical forces and physical couples,

$$\operatorname{Div}\mathbf{T}+\mathbf{b}=\dot{\mathbf{p}},\quad \mathbf{T}\mathbf{F}^{\mathrm{T}}-\mathbf{F}\mathbf{T}^{\mathrm{T}}=\mathbf{0}, \tag{2.16}$$

where $(2.16)_2$ represents the symmetry condition of the second Piola–Kirchhoff and Cauchy stress tensor, respectively.

Correspondingly, from (2.15) we derive the set of local balance laws of material forces,

$$\operatorname{Div}\boldsymbol{\Sigma}-\boldsymbol{\sigma}+\boldsymbol{\beta}=\dot{\boldsymbol{\pi}}, \tag{2.17}$$

representing three independent weakly-nonlocal material force balances. They are also independent of the physical force balance $(2.16)_1$.

In the global material forces balance (2.15) there may be singular surfaces with material forces acting on these surfaces, then the corresponding jump conditions of the material forces on these surfaces have to be added to (2.17).

2.5. Principle of virtual power

To derive the principle of virtual power corresponding to the physical and material balance laws $(2.16)_1$ and (2.17), we formulate their weak form. For every part P of the material body and arbitrary vector-valued physical velocity field $\mathbf{v}(\mathbf{X},t)$ and arbitrary tensor-valued material velocity fields $\boldsymbol{v}(\mathbf{X},t)$, defined as ordered set

$$\boldsymbol{v}(\mathbf{X},t)=\left\{\mathbf{V}^{\mathrm{d}}(\mathbf{X},t),\mathbf{V}^{\mathrm{p}}(\mathbf{X},t),\mathbf{v}^{\mathrm{p}}(\mathbf{X},t)\right\}, \tag{2.18}$$

a direct implication of $(2.16)_1$ and (2.17) together with possible jump conditions is

$$\int_P\left((\operatorname{Div}\mathbf{T}+\mathbf{b}-\dot{\mathbf{p}})\bullet\mathbf{v}+(\operatorname{Div}\boldsymbol{\Sigma}-\boldsymbol{\sigma}+\boldsymbol{\beta}-\dot{\boldsymbol{\pi}})\bullet\boldsymbol{v}\right)\mathrm{d}v=0. \tag{2.19}$$

The use of the divergence theorem allows us to rewrite Eq. (2.19) in the form

$$\begin{aligned}&\int_P(\dot{\mathbf{p}}\bullet\mathbf{v}+\dot{\boldsymbol{\pi}}\bullet\boldsymbol{v})\,\mathrm{d}v+\int_P(\mathbf{T}\bullet\nabla\mathbf{v}+\boldsymbol{\sigma}\bullet\boldsymbol{v}+\boldsymbol{\Sigma}\bullet\nabla\boldsymbol{v})\,\mathrm{d}v\\&\quad=\int_P(\mathbf{b}\bullet\mathbf{v}+\boldsymbol{\beta}\bullet\boldsymbol{v})\,\mathrm{d}v+\int_{\partial P}(\mathbf{T}\mathbf{n}\bullet\mathbf{v}+\boldsymbol{\Sigma}\mathbf{n}\bullet\boldsymbol{v})\,\mathrm{d}a.\end{aligned} \tag{2.20}$$

Eq. (2.20) expresses the integral laws and hence also local laws of physical and material linear momenta in the weak form representing the principle of virtual power for physical and material space.

Reversing the derivation outlined above it is easily seen that the local Eqs. $(2.16)_1$ and (2.17) can be derived also taking the principle of virtual power (2.20) as the basic postulate instead of the integral balance laws (2.11) and (2.15). Moreover, it is obvious that the principle (2.20) applies also to the whole body B. In this case, the inspection of the boundary integral in (2.20) naturally leads to a consistent formulation of the boundary conditions (Stumpf and Hackl, 2003).

Taking the virtual physical and material kinematical variables to be real velocities, $\mathbf{v}=\dot{\mathbf{x}}$, $\boldsymbol{v}=\dot{\boldsymbol{\varepsilon}}$, the principle of virtual power (2.20) can be rewritten as

$$\begin{aligned}&\int_P(\dot{\mathbf{p}}\bullet\dot{\mathbf{x}}+\dot{\boldsymbol{\pi}}\bullet\dot{\boldsymbol{\varepsilon}})\,\mathrm{d}v+\int_P(\mathbf{T}\bullet\nabla\dot{\mathbf{x}}+\boldsymbol{\sigma}\bullet\dot{\boldsymbol{\varepsilon}}+\boldsymbol{\Sigma}\bullet\nabla\dot{\boldsymbol{\varepsilon}})\,\mathrm{d}v\\&\quad=\int_P(\mathbf{b}\bullet\dot{\mathbf{x}}+\boldsymbol{\beta}\bullet\dot{\boldsymbol{\varepsilon}})\,\mathrm{d}v+\int_{\partial P}(\mathbf{T}\mathbf{n}\bullet\dot{\mathbf{x}}+\boldsymbol{\Sigma}\mathbf{n}\bullet\dot{\boldsymbol{\varepsilon}})\,\mathrm{d}a.\end{aligned} \tag{2.21}$$

With appropriate assumptions concerning the linear momenta in the physical and material space (see Stumpf and Hackl, 2003), the first integral of (2.21) can be transformed to

$$\int_P(\dot{\mathbf{p}}\bullet\dot{\mathbf{x}}+\dot{\boldsymbol{\pi}}\bullet\dot{\boldsymbol{\varepsilon}})\,\mathrm{d}v=\frac{\mathrm{d}}{\mathrm{d}t}\int_P\kappa(\dot{\mathbf{x}},\dot{\boldsymbol{\varepsilon}})\,\mathrm{d}v, \tag{2.22}$$

where $\kappa(\dot{\mathbf{x}}, \dot{\mathbf{F}}^{\mathrm{d}}, \dot{\mathbf{F}}^{\mathrm{p}}, \dot{\xi}^{\mathrm{p}})$ is the kinetic energy density in physical and material space,

$$\kappa(\dot{\mathbf{x}}, \dot{\boldsymbol{\varepsilon}}) = \frac{1}{2}\rho_0(\dot{\mathbf{x}} \bullet \dot{\mathbf{x}} + \mathsf{J}\dot{\boldsymbol{\varepsilon}} \bullet \dot{\boldsymbol{\varepsilon}}), \tag{2.23}$$

with $\dot{\boldsymbol{\varepsilon}}$ defined by (2.7), and J is an ordered set of fourth and second order, respectively, material microinertia tensors denoted as

$$\mathsf{J} = \{\mathsf{J}^{\mathrm{d}}, \mathsf{J}^{\mathrm{p}}, \mathbf{J}^{\mathrm{p}}\}. \tag{2.24}$$

With (2.7) and (2.24) the kinetic energy of physical and material space (2.23) is given as

$$\kappa(\dot{\mathbf{x}}, \dot{\mathbf{F}}^{\mathrm{d}}, \dot{\mathbf{F}}^{\mathrm{p}}, \dot{\xi}^{\mathrm{p}}) = \frac{1}{2}\rho_0\left(\dot{\mathbf{x}} \bullet \dot{\mathbf{x}} + \mathsf{J}^{\mathrm{d}}\dot{\mathbf{F}}^{\mathrm{d}} \bullet \dot{\mathbf{F}}^{\mathrm{d}} + \mathsf{J}^{\mathrm{p}}\dot{\mathbf{F}}^{\mathrm{p}} \bullet \dot{\mathbf{F}}^{\mathrm{p}} + \mathbf{J}^{\mathrm{p}}\dot{\xi}^{\mathrm{p}} \bullet \dot{\xi}^{\mathrm{p}}\right). \tag{2.25}$$

The fourth and second order material microinertia tensors J^{d}, J^{p} and $\mathbf{J}^{\mathrm{p}}$ have to satisfy certain symmetry conditions in order to ensure that the kinetic energy (2.25) serves as potential of the material momenta $\mathbf{P}^{\mathrm{d}}$, $\mathbf{P}^{\mathrm{p}}$ and $\mathbf{p}^{\mathrm{p}}$. Such conditions are satisfied identically, if the inertia tensors (2.24) are symmetric and time independent. Then it follows:

$$\begin{aligned}
\mathbf{p} &= \frac{\partial\kappa(\dot{\mathbf{x}}, \dot{\mathbf{F}}^{\mathrm{d}}, \dot{\mathbf{F}}^{\mathrm{p}}, \dot{\xi}^{\mathrm{p}})}{\partial\dot{\mathbf{x}}}\Big|_{\dot{\mathbf{F}}^{\mathrm{d}}, \dot{\mathbf{F}}^{\mathrm{p}}, \dot{\xi}^{\mathrm{p}}} = \rho_0\dot{\mathbf{x}},\\
\mathbf{P}^{\mathrm{d}} &= \frac{\partial\kappa(\dot{\mathbf{x}}, \dot{\mathbf{F}}^{\mathrm{d}}, \dot{\mathbf{F}}^{\mathrm{p}}, \dot{\xi}^{\mathrm{p}})}{\partial\dot{\mathbf{F}}^{\mathrm{d}}}\Big|_{\dot{\mathbf{x}}, \dot{\mathbf{F}}^{\mathrm{p}}, \dot{\xi}^{\mathrm{p}}} = \rho_0\mathsf{J}^{\mathrm{d}}\dot{\mathbf{F}}^{\mathrm{d}},\\
\mathbf{P}^{\mathrm{p}} &= \frac{\partial\kappa(\dot{\mathbf{x}}, \dot{\mathbf{F}}^{\mathrm{d}}, \dot{\mathbf{F}}^{\mathrm{p}}, \dot{\xi}^{\mathrm{p}})}{\partial\dot{\mathbf{F}}^{\mathrm{p}}}\Big|_{\dot{\mathbf{x}}, \dot{\mathbf{F}}^{\mathrm{d}}, \dot{\xi}^{\mathrm{p}}} = \rho_0\mathsf{J}^{\mathrm{p}}\dot{\mathbf{F}}^{\mathrm{p}},\\
\mathbf{p}^{\mathrm{p}} &= \frac{\partial\kappa(\dot{\mathbf{x}}, \dot{\mathbf{F}}^{\mathrm{d}}, \dot{\mathbf{F}}^{\mathrm{p}}, \dot{\xi}^{\mathrm{p}})}{\partial\dot{\xi}^{\mathrm{p}}}\Big|_{\dot{\mathbf{x}}, \dot{\mathbf{F}}^{\mathrm{d}}, \dot{\mathbf{F}}^{\mathrm{p}}} = \rho_0\mathbf{J}^{\mathrm{p}}\dot{\xi}^{\mathrm{p}},
\end{aligned} \tag{2.26}$$

where the variables behind a stroke have to be kept constant. The form (2.25) of the kinetic energy of dynamically evolving defects is assumed following results of Naghdi and Srinivasa (1993a) and Le and Stumpf (1996b) on dislocation dynamics without hardening.

With (2.25) and (2.26), Eq. (2.21) with (2.22) can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_P \kappa\,\mathrm{d}v + \int_P \sigma\,\mathrm{d}v = \int_P (\mathbf{b} \bullet \dot{\mathbf{x}} + \boldsymbol{\beta} \bullet \dot{\boldsymbol{\varepsilon}})\,\mathrm{d}v + \int_{\partial P} (\mathbf{T}\mathbf{n} \bullet \dot{\mathbf{x}} + \boldsymbol{\Sigma}\mathbf{n} \bullet \dot{\boldsymbol{\varepsilon}})\,\mathrm{d}a, \tag{2.27}$$

where the stress power density σ of physical and material forces and stresses is obtained as

$$\sigma \equiv \mathbf{T} \bullet \dot{\mathbf{F}} + \boldsymbol{\sigma} \bullet \dot{\boldsymbol{\varepsilon}} + \boldsymbol{\Sigma} \bullet \nabla\dot{\boldsymbol{\varepsilon}}. \tag{2.28}$$

2.6. Integral and local forms of first and second law of thermodynamics

A reliable formulation of the constitutive equations for irreversible processes of deformable material bodies undergoing damage and plastic deformations requires a fully thermodynamical theory for deformation in the physical space and defect and plastic evolution as well as heat flux in the material space. This requires additionally to the global balance laws of physical forces and couples (2.11), (2.12) and material forces (2.15) an appropriate global formulation of the first and second law of thermodynamics for physical and material space.

Taking into account the results derived in the previous section, the first law of thermodynamics expressing the balance of energy for physical and material space takes the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_P(\varepsilon+\kappa)\,\mathrm{d}v=\int_P(\mathbf{b}\bullet\dot{\mathbf{x}}+\boldsymbol{\beta}\bullet\dot{\boldsymbol{\varepsilon}})\,\mathrm{d}v+\int_{\partial P}(\mathbf{T}\mathbf{n}\bullet\dot{\mathbf{x}}+\boldsymbol{\Sigma}\mathbf{n}\bullet\dot{\boldsymbol{\varepsilon}})\,\mathrm{d}a+\int_P r\,\mathrm{d}v-\int_{\partial P}\mathbf{q}\bullet\mathbf{n}\,\mathrm{d}a. \tag{2.29}$$

Here, $\varepsilon(\mathbf{X},t)$ denotes the internal energy, $\kappa(\mathbf{X},t)$ the kinetic energy (2.25), $r(\mathbf{X},t)$ the heat source and $\mathbf{q}(\mathbf{X},t)$ the heat flux vector.

The second law of thermodynamics expresses the principle of entropy growth and its general form is

$$\int_P \mathrm{d}\,\mathrm{d}v\equiv\frac{\mathrm{d}}{\mathrm{d}t}\int_P\eta\,\mathrm{d}v-\int_P\theta^{-1}r\,\mathrm{d}v+\int_{\partial P}(\theta^{-1}\mathbf{q})\bullet\mathbf{n}\,\mathrm{d}a\geqslant 0, \tag{2.30}$$

where $\mathrm{d}(\mathbf{X},t)$ is the energy dissipation per reference volume, $\eta(\mathbf{X},t)$ the specific entropy and $\theta(\mathbf{X},t)>0$ the absolute temperature.

Under the assumption that the balances of physical and material forces (2.11) and (2.15) are satisfied, the localization of the balance law of energy (2.29) yield the local equation

$$\dot{\varepsilon}=\sigma+r-\mathrm{Div}\,\mathbf{q}, \tag{2.31}$$

where σ is the stress power density given by (2.28). Moreover, the localization of the second law of thermodynamics (2.30) yields the inequality

$$\mathrm{d}\equiv\dot{\eta}-\theta^{-1}r+\mathrm{Div}(\theta^{-1}\mathbf{q})\geqslant 0. \tag{2.32}$$

With the use of the local energy balance (2.31) and the definition of the free energy $\psi(\mathbf{X},t)$,

$$\psi\equiv\varepsilon-\theta\eta, \tag{2.33}$$

the term $r-\mathrm{Div}\,\mathbf{q}$ may be eliminated from (2.32) to give the local dissipation inequality in the form

$$\mathrm{d}\equiv\sigma-\eta\dot{\theta}-\theta^{-1}\mathbf{q}\bullet\nabla\theta-\dot{\psi}\geqslant 0. \tag{2.34}$$

The derivation of a fully thermodynamical theory may follow the procedure outlined in Stumpf and Hackl (2003).

2.7. Local dissipation inequality for isothermal processes

In this paper we restrict our subsequent considerations to isothermal processes. Then the dissipation inequality (2.34) reduces to the form

$$\mathrm{d}\equiv\sigma-\dot{\psi}\geqslant 0, \tag{2.35}$$

and with the stress power due to (2.28) to

$$\mathrm{d}\equiv\mathbf{T}\bullet\dot{\mathbf{F}}+\mathbf{T}^{\mathrm{d}}\bullet\dot{\mathbf{F}}^{\mathrm{d}}+\mathrm{H}^{\mathrm{d}}\bullet\nabla\dot{\mathbf{F}}^{\mathrm{d}}+\mathbf{T}^{\mathrm{p}}\bullet\dot{\mathbf{F}}^{\mathrm{p}}+\mathrm{H}^{\mathrm{p}}\bullet\nabla\dot{\mathbf{F}}^{\mathrm{p}}+\mathbf{t}^{\mathrm{p}}\bullet\dot{\xi}^{\mathrm{p}}+\mathbf{H}^{\mathrm{p}}\bullet\nabla\dot{\xi}^{\mathrm{p}}-\dot{\psi}\geqslant 0. \tag{2.36}$$

The inequality (2.36) represents the second law of thermodynamics for isothermal processes under the assumption that the balance laws of physical and material forces hold.

3. Thermodynamically consistent constitutive equations for isothermal processes and governing equations

3.1. Consequences of the second law of thermodynamics

We assume the general constitutive form of free energy ψ, physical stress tensor $\mathbf{T}$, material stress tensors $\boldsymbol{\sigma}$ according to (2.8) and material stress tensors $\boldsymbol{\Sigma}$ due to (2.9) as follows:

$$\begin{aligned}
\psi &= \hat{\psi}(\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \dot{\mathbf{F}}, \dot{\boldsymbol{\varepsilon}}, \nabla\dot{\boldsymbol{\varepsilon}}),\\
\mathbf{T} &= \hat{\mathbf{T}}(\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \dot{\mathbf{F}}, \dot{\boldsymbol{\varepsilon}}, \nabla\dot{\boldsymbol{\varepsilon}}),\\
\boldsymbol{\sigma} &= \hat{\boldsymbol{\sigma}}(\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \dot{\mathbf{F}}, \dot{\boldsymbol{\varepsilon}}, \nabla\dot{\boldsymbol{\varepsilon}}),\\
\boldsymbol{\Sigma} &= \hat{\boldsymbol{\Sigma}}(\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \dot{\mathbf{F}}, \dot{\boldsymbol{\varepsilon}}, \nabla\dot{\boldsymbol{\varepsilon}}).
\end{aligned} \tag{3.1}$$

Introducing (3.1) into the second law (2.36) leads to the thermodynamically admissible form of the constitutive equations, where the free energy has to satisfy the restrictions

$$\partial_{\dot{\mathbf{F}}}\hat{\psi} = \mathbf{0}, \quad \partial_{\dot{\boldsymbol{\varepsilon}}}\hat{\psi} = \mathbf{0}, \quad \partial_{\nabla\dot{\boldsymbol{\varepsilon}}}\hat{\psi} = \mathbf{0}, \tag{3.2}$$

it means that the free energy may be of the form

$$\psi = \hat{\psi}(\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}) \tag{3.3}$$

and cannot depend on the rates $\dot{\mathbf{F}}$, $\dot{\boldsymbol{\varepsilon}}$, $\nabla\dot{\boldsymbol{\varepsilon}}$.

With (3.1) and in view of (3.3) the dissipation inequality (2.36) reduces to

$$\begin{aligned}
\mathsf{d} = &\left(\hat{\mathbf{T}}(\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \dot{\mathbf{F}}, \dot{\boldsymbol{\varepsilon}}, \nabla\dot{\boldsymbol{\varepsilon}}) - \partial_{\mathbf{F}}\hat{\psi}(\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon})\right) \bullet \dot{\mathbf{F}} + \left(\hat{\boldsymbol{\sigma}}(\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \dot{\mathbf{F}}, \dot{\boldsymbol{\varepsilon}}, \nabla\dot{\boldsymbol{\varepsilon}}) - \partial_{\boldsymbol{\varepsilon}}\hat{\psi}(\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon})\right) \bullet \dot{\boldsymbol{\varepsilon}}\\
&+ \left(\hat{\boldsymbol{\Sigma}}(\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \dot{\mathbf{F}}, \dot{\boldsymbol{\varepsilon}}, \nabla\dot{\boldsymbol{\varepsilon}}) - \partial_{\nabla\boldsymbol{\varepsilon}}\hat{\psi}(\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon})\right) \bullet \nabla\dot{\boldsymbol{\varepsilon}} \geqslant 0.
\end{aligned} \tag{3.4}$$

The inspection of (3.4) leads to the result that the physical and material stresses consist of two parts, a non-dissipative part, which can be derived from a free energy potential ψ, and a dissipative part, which is indicated here by a lower asterisk,

$$\begin{aligned}
\mathbf{T} &= \partial_{\mathbf{F}}\hat{\psi}(\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}) + \hat{\mathbf{T}}_*(\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \dot{\mathbf{F}}, \dot{\boldsymbol{\varepsilon}}, \nabla\dot{\boldsymbol{\varepsilon}}),\\
\boldsymbol{\sigma} &= \partial_{\boldsymbol{\varepsilon}}\hat{\psi}(\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}) + \hat{\boldsymbol{\sigma}}_*(\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \dot{\mathbf{F}}, \dot{\boldsymbol{\varepsilon}}, \nabla\dot{\boldsymbol{\varepsilon}}),\\
\boldsymbol{\Sigma} &= \partial_{\nabla\boldsymbol{\varepsilon}}\hat{\psi}(\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}) + \hat{\boldsymbol{\Sigma}}_*(\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \dot{\mathbf{F}}, \dot{\boldsymbol{\varepsilon}}, \nabla\dot{\boldsymbol{\varepsilon}}),
\end{aligned} \tag{3.5}$$

where the dissipative parts of the physical and material stresses have to satisfy the dissipation inequality in the form,

$$\mathsf{d} = \hat{\mathbf{T}}_*(\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \dot{\mathbf{F}}, \dot{\boldsymbol{\varepsilon}}, \nabla\dot{\boldsymbol{\varepsilon}}) \bullet \dot{\mathbf{F}} + \hat{\boldsymbol{\sigma}}_*(\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \dot{\mathbf{F}}, \dot{\boldsymbol{\varepsilon}}, \nabla\dot{\boldsymbol{\varepsilon}}) \bullet \dot{\boldsymbol{\varepsilon}} + \hat{\boldsymbol{\Sigma}}_*(\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \dot{\mathbf{F}}, \dot{\boldsymbol{\varepsilon}}, \nabla\dot{\boldsymbol{\varepsilon}}) \bullet \nabla\dot{\boldsymbol{\varepsilon}} \geqslant 0. \tag{3.6}$$

In (3.6) the first term represents the dissipation due to viscous effects on the macrolevel, the second term the dissipation due to the local driving forces on defects and dislocations in the material space and the third term their additional weakly-nonlocal contribution.

To complete the set of constitutive equations, we have to add criteria of the initiation of damage and plastic flow, usually denoted as threshold value and yield condition, respectively. Here we assume two independent scalar-valued criteria of the form,

$$f^{\mathrm{d}} = f^{\mathrm{d}}(\mathbf{T}, \boldsymbol{\sigma}, \boldsymbol{\Sigma}; \mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}) \leqslant 0, \quad f^{\mathrm{p}} = f^{\mathrm{p}}(\mathbf{T}, \boldsymbol{\sigma}, \boldsymbol{\Sigma}; \mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}) \leqslant 0, \tag{3.7}$$

where the stresses $\{\mathbf{T}, \boldsymbol{\sigma}, \boldsymbol{\Sigma}\}$ in the initiation conditions (3.7) are the non-dissipative equilibrium parts of (3.5) defined by the first terms on the right side. A special case of $(3.7)_2$ is considered in Sluys et al. (1993) for gradient elastoplasticity at small strains. Their yield condition depends on the stress tensor, the plastic equivalent strain and its second gradient.

To simplify the notation scheme furthermore, we collect the physical and material kinematical variables and their rates in the ordered sets

$$\mathbf{e} = \{\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}\}, \quad \dot{\mathbf{e}} = \{\dot{\mathbf{F}}, \dot{\boldsymbol{\varepsilon}}, \nabla\dot{\boldsymbol{\varepsilon}}\} \tag{3.8}$$

and the physical and material forces in the ordered set

$$\mathbf{s} = \{\mathbf{T}, \boldsymbol{\sigma}, \boldsymbol{\Sigma}\}. \tag{3.9}$$

The ordered set

$$\mathbf{e}(\mathbf{X}, t) = \{\mathbf{e}, \dot{\mathbf{e}}\}(\mathbf{X}, t) = \{\mathbf{F}, \boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \dot{\mathbf{F}}, \dot{\boldsymbol{\varepsilon}}, \nabla\dot{\boldsymbol{\varepsilon}}\}(\mathbf{X}, t), \tag{3.10}$$

with $\boldsymbol{\varepsilon}$ according to (2.5), defines the state space of our theory with the independent kinematical variables. It should be pointed out that at one point the values of the fields and the gradients are independent variables. The independency of the values of the fields and their gradients is only locally true.

By making the space gradients of the state space (3.10) dimensionless additional material parameters can be introduced into the theory, which have the dimension of lengths. In this way length scales are included in the theory causing localization zones to have a finite width and not to collapse into discontinuities. For details in gradient-enhanced elastoplasticity at small strains and numerical consequences the reader may refer to de Borst et al. (1993), Sluys et al. (1993) and de Borst (2001). In the latter paper it is shown how internal length scales can be backtraced from experimental data. To make also the rates and time gradients, respectively, dimensionless, also a time scale may be introduced in the state space (3.10).

With (3.10) the constitutive equations (3.5) can be written as

$$\begin{aligned} \mathbf{T} &= \partial_{\mathbf{F}}\hat{\psi}(\mathbf{e}) + \hat{\mathbf{T}}_*(\mathbf{e}, \dot{\mathbf{e}}), \\ \boldsymbol{\sigma} &= \partial_{\boldsymbol{\varepsilon}}\hat{\psi}(\mathbf{e}) + \hat{\boldsymbol{\sigma}}_*(\mathbf{e}, \dot{\mathbf{e}}), \\ \boldsymbol{\Sigma} &= \partial_{\nabla\boldsymbol{\varepsilon}}\hat{\psi}(\mathbf{e}) + \hat{\boldsymbol{\Sigma}}_*(\mathbf{e}, \dot{\mathbf{e}}), \end{aligned} \tag{3.11}$$

or, equivalently, in set form

$$\mathbf{s} = \partial_{\mathbf{e}}\hat{\psi}(\mathbf{e}) + \hat{\mathbf{s}}_*(\mathbf{e}, \dot{\mathbf{e}}) \tag{3.12}$$

with the set of dissipative driving forces

$$\mathbf{s}_* = \hat{\mathbf{s}}_*(\mathbf{e}, \dot{\mathbf{e}}) = \{\hat{\mathbf{T}}_*(\mathbf{e}, \dot{\mathbf{e}}), \hat{\boldsymbol{\sigma}}_*(\mathbf{e}, \dot{\mathbf{e}}), \hat{\boldsymbol{\Sigma}}_*(\mathbf{e}, \dot{\mathbf{e}})\}. \tag{3.13}$$

With (3.13) the dissipation inequality (3.6) reads

$$\mathsf{d} = \hat{\mathbf{s}}_*(\mathbf{e}, \dot{\mathbf{e}}) \bullet \dot{\mathbf{e}} \geqslant 0, \tag{3.14}$$

describing the rate of entropy growth.

In general, the one-form (3.14) need not be integrable. However, if it is integrable then there exists a scalar-valued function φ of the form $\varphi = \hat{\varphi}(\mathbf{e}, \dot{\mathbf{e}})$ such that

$$\mathsf{d}(\mathbf{e}, \dot{\mathbf{e}}) = \mathrm{d}\hat{\varphi}(\mathbf{e}, \dot{\mathbf{e}}) = (\partial_{\dot{\mathbf{e}}}\hat{\varphi}(\mathbf{e}, \dot{\mathbf{e}})) \bullet \dot{\mathbf{e}}, \tag{3.15}$$

where $\hat{\varphi}(\mathbf{e}, \dot{\mathbf{e}})$ is a dissipation pseudo-potential, which enables to express the dissipative driving stresses (3.13) by one functional

$$\mathbf{s}_*(\mathbf{e}, \dot{\mathbf{e}}) = \partial_{\dot{\mathbf{e}}}\hat{\varphi}(\mathbf{e}, \dot{\mathbf{e}}). \tag{3.16}$$

Introducing (3.16) into (3.12) leads to the thermodynamically consistent constitutive equations

$$\mathbf{s} = \partial_{\mathbf{e}}\hat{\psi}(\mathbf{e}) + \partial_{\dot{\mathbf{e}}}\hat{\varphi}(\mathbf{e}, \dot{\mathbf{e}}) \tag{3.17}$$

and the dissipation inequality

$$\mathsf{d}(\mathbf{e}, \dot{\mathbf{e}}) = \hat{\mathbf{s}}_*(\mathbf{e}, \dot{\mathbf{e}}) \bullet \dot{\mathbf{e}} = \partial_{\dot{\mathbf{e}}}\hat{\varphi}(\mathbf{e}, \dot{\mathbf{e}}) \bullet \dot{\mathbf{e}} \geqslant 0. \tag{3.18}$$

3.2. Semi-linear form of the driving forces

Whether the one-form (3.14) is integrable or not depends on the particular form of the response functions of the dissipative stresses (3.13). In order to give an illustration of this point let us assume that the response functions (3.13) are linear with respect to the rates $\dot{\mathbf{e}}$,

$$\mathbf{s}_*(\mathbf{e},\dot{\mathbf{e}}) = \mathbf{L}(\mathbf{e})\dot{\mathbf{e}}. \tag{3.19}$$

Introducing the semi-linear constitutive equation (3.19) into the dissipation inequality (3.18) leads to

$$\mathrm{d}(\mathbf{e},\dot{\mathbf{e}}) = \mathbf{s}_*(\mathbf{e},\dot{\mathbf{e}}) \bullet \dot{\mathbf{e}} = (\mathbf{L}(\mathbf{e})\dot{\mathbf{e}}) \bullet \dot{\mathbf{e}} = \mathbf{L}(\mathbf{e}) \bullet (\dot{\mathbf{e}} \otimes \dot{\mathbf{e}}) \geqslant 0, \tag{3.20}$$

where the tensor product of vectors and tensors are defined in the usual way.

Let us assume that the constitutive operator $\mathbf{L}(\mathbf{e})$ may be written as sum of a symmetric and a skew-symmetric part,

$$\mathbf{L}(\mathbf{e}) = \mathbf{L}_{\mathrm{S}}(\mathbf{e}) + \mathbf{L}_{\mathrm{skw}}(\mathbf{e}). \tag{3.21}$$

If the skew-symmetric part vanishes, $\mathbf{L}_{\mathrm{skw}}(\mathbf{e}) = \mathbf{0}$, then the entropy growth $\mathrm{d}(\mathbf{e},\dot{\mathbf{e}})$ given by (3.20) is integrable leading to a dissipation pseudo-potential of the form

$$\varphi(\mathbf{e},\dot{\mathbf{e}}) = \mathbf{L}_{\mathrm{S}}(\mathbf{e}) \bullet (\dot{\mathbf{e}} \otimes \dot{\mathbf{e}}) = \frac{1}{2}\left(\mathbf{L}(\mathbf{e}) + \mathbf{L}(\mathbf{e})^{\mathrm{T}}\right) \bullet (\dot{\mathbf{e}} \otimes \dot{\mathbf{e}}). \tag{3.22}$$

With the dissipation pseudo-potential (3.22) the constitutive equation (3.17) are obtained as

$$\mathbf{s}(\mathbf{e},\dot{\mathbf{e}}) = \partial_{\mathbf{e}}\psi(\mathbf{e}) + \partial_{\dot{\mathbf{e}}}\varphi(\mathbf{e},\dot{\mathbf{e}}) = \partial_{\mathbf{e}}\psi(\mathbf{e}) + \mathbf{L}_{\mathrm{S}}(\mathbf{e})\dot{\mathbf{e}}. \tag{3.23}$$

3.3. Extremal properties of the entropy production

As noted above, the properties of the dissipation pseudo-potential depend on the properties of the response functions of the dissipative stresses. In the particular case of semi-linear response functions, such properties are determined by the properties of the constitutive operator $\mathbf{L}_{\mathrm{S}}(\mathbf{e})$. In general, the dissipation pseudo-potential given by the quadratic form (3.22) is semi-positive definite, i.e.

$$\varphi(\mathbf{e},\dot{\mathbf{e}}) = \mathbf{L}_{\mathrm{S}}(\mathbf{e}) \bullet (\dot{\mathbf{e}} \otimes \dot{\mathbf{e}}) \geqslant 0, \quad \varphi(\mathbf{e},\mathbf{0}) = 0 \tag{3.24}$$

for all $\dot{\mathbf{e}}$, and it takes zero value at the equilibrium state $\dot{\mathbf{e}} = \mathbf{0}$. If the operator $\mathbf{L}_{\mathrm{S}}(\mathbf{e})$ is non-singular, then the relation (3.19) can be inverted yielding

$$\dot{\mathbf{e}} = \mathbf{L}_{\mathrm{S}}(\mathbf{e})^{-1}\mathbf{s}_*. \tag{3.25}$$

If in addition the constitutive operator $\mathbf{L}_{\mathrm{S}}(\mathbf{e})$ is positive definite, then the dissipation pseudo-potential given by the quadratic form (3.22) has the minimum at the equilibrium state $\dot{\mathbf{e}} = \mathbf{0}$ and this minimum is zero.

3.4. Governing equations for isothermal dissipative processes

The governing equations determining the dissipative deformation process with defect and plastic evolution are obtained by introducing the constitutive equation (3.17) into the physical force balance $(2.16)_1$ and the material force balance (2.17) with (2.14) and (2.26), yielding the set of equations

$$\mathrm{Div}(\partial_{\mathbf{F}}\hat{\psi}(\mathbf{e}) + \partial_{\dot{\mathbf{F}}}\hat{\varphi}(\mathbf{e},\dot{\mathbf{e}})) + \mathbf{b} = \rho_0\ddot{\mathbf{x}}, \tag{3.26}$$

$$\begin{aligned}
&\mathrm{Div}\Big(\partial_{\nabla\mathbf{F}^{\mathrm{d}}}\hat{\psi}(\mathbf{e})+\partial_{\nabla\dot{\mathbf{F}}^{\mathrm{d}}}\hat{\varphi}(\mathbf{e},\dot{\mathbf{e}})\Big)-\Big(\partial_{\mathbf{F}^{\mathrm{d}}}\hat{\psi}(\mathbf{e})+\partial_{\dot{\mathbf{F}}^{\mathrm{d}}}\hat{\varphi}(\mathbf{e},\dot{\mathbf{e}})\Big)+\mathbf{G}^{\mathrm{d}}=\rho_0(\mathrm{J}^{\mathrm{d}}\dot{\mathbf{F}}^{\mathrm{d}})^{\bullet},\\
&\mathrm{Div}\Big(\partial_{\nabla\mathbf{F}^{\mathrm{p}}}\hat{\psi}(\mathbf{e})+\partial_{\nabla\dot{\mathbf{F}}^{\mathrm{p}}}\hat{\varphi}(\mathbf{e},\dot{\mathbf{e}})\Big)-\Big(\partial_{\mathbf{F}^{\mathrm{p}}}\hat{\psi}(\mathbf{e})+\partial_{\dot{\mathbf{F}}^{\mathrm{p}}}\hat{\varphi}(\mathbf{e},\dot{\mathbf{e}})\Big)+\mathbf{G}^{\mathrm{p}}=\rho_0(\mathrm{J}^{\mathrm{p}}\dot{\mathbf{F}}^{\mathrm{p}})^{\bullet},\\
&\mathrm{Div}\Big(\partial_{\nabla\xi^{\mathrm{p}}}\hat{\psi}(\mathbf{e})+\partial_{\nabla\dot{\xi}^{\mathrm{p}}}\hat{\varphi}(\mathbf{e},\dot{\mathbf{e}})\Big)-\Big(\partial_{\xi^{\mathrm{p}}}\hat{\psi}(\mathbf{e})+\partial_{\dot{\xi}^{\mathrm{p}}}\hat{\varphi}(\mathbf{e},\dot{\mathbf{e}})\Big)+\mathbf{g}^{\mathrm{p}}=\rho_0(\mathbf{J}^{\mathrm{p}}\dot{\xi}^{\mathrm{p}})^{\bullet},
\end{aligned}\tag{3.27}$$

where $\mathbf{e}$ is the set of physical and material kinematical variables according to $(3.8)_1$,

$$\mathbf{e}=\{\mathbf{F},\mathbf{F}^{\mathrm{d}},\mathbf{F}^{\mathrm{p}},\xi^{\mathrm{p}},\nabla\mathbf{F}^{\mathrm{d}},\nabla\mathbf{F}^{\mathrm{p}},\nabla\xi^{\mathrm{p}}\}.\tag{3.28}$$

Since the kinematical variables (3.28) and their rates are not objective, we have to replace them by their objective counterparts, which can be obtained easily by pull-back to the undeformed and homogeneous reference configuration (see e.g. Stumpf and Hoppe, 1997).

To determine dissipative deformation processes with defect evolution and dislocation motion the governing Eqs. (3.26) and (3.27) have to be supplemented by corresponding boundary and initial conditions (see Stumpf and Hackl, 2003) and activation criteria for damage and plastic flow of the form (3.7), where the dissipative process has to satisfy the dissipation inequality (3.14) and (3.18), respectively.

With (3.26) and (3.27) we have as many equations as we have independent unknown fields, $\{\mathbf{F},\mathbf{F}^{\mathrm{d}},\mathbf{F}^{\mathrm{p}},\xi^{\mathrm{p}}\}(\mathbf{X},t)$, and since the set of equations discussed above is complete, we are able to determine the unknown fields. Of course, the result depends essentially on the constitutive equations of the specific problem under consideration. Global uniqueness of the solution should be proved following the methodology presented recently by Mosconi (in press) for gradient models of brittle damage.

In our considerations so far we assumed that the free energy $\psi=\hat{\psi}(\mathbf{e})$ and the dissipation pseudo-potential $\varphi=\hat{\varphi}(\mathbf{e},\dot{\mathbf{e}})$ are differentiable functions. This is not the case at yield and damage activation points, where differentiability in the classical sense is not given and has to be replaced by the notion of subdifferentiability (Moreau, 1970). For simplicity we do not introduce here the usual symbols of subdifferentiation.

4. Simplified gradient and local theories for quasi-static deformation

4.1. Neglecting viscous effects on the macrolevel and nonlocal rate contributions on meso- and microlevel

If we assume that $\dot{\mathbf{F}}$, $\nabla\dot{\mathbf{F}}^{\mathrm{d}}$, $\nabla\dot{\mathbf{F}}^{\mathrm{p}}$ and $\nabla\dot{\xi}^{\mathrm{p}}$ can be neglected,

$$\dot{\mathbf{F}}=\mathbf{0},\quad \nabla\dot{\mathbf{F}}^{\mathrm{d}}=\mathbf{0},\quad \nabla\dot{\mathbf{F}}^{\mathrm{p}}=\mathbf{0},\quad \nabla\dot{\xi}^{\mathrm{p}}=\mathbf{0},\tag{4.1}$$

then far simpler weakly-nonlocal models of damage and finite elastoplasticity are obtained, where the free energy and the dissipation pseudo-potential take the form

$$\psi=\hat{\psi}(\mathbf{e}),\quad \varphi=\hat{\varphi}(\mathbf{e},\dot{\mathbf{F}}^{\mathrm{d}},\dot{\mathbf{F}}^{\mathrm{p}},\dot{\xi}^{\mathrm{p}}),\tag{4.2}$$

with $\mathbf{e}$ given by (3.28). The dissipation inequality following from (3.18) leads to

$$\mathrm{d}=\partial_{\dot{\mathbf{F}}^{\mathrm{d}}}\hat{\varphi}\bullet\dot{\mathbf{F}}^{\mathrm{d}}+\partial_{\dot{\mathbf{F}}^{\mathrm{p}}}\hat{\varphi}\bullet\dot{\mathbf{F}}^{\mathrm{p}}+\partial_{\dot{\xi}^{\mathrm{p}}}\hat{\varphi}\bullet\dot{\xi}^{\mathrm{p}}\geqslant 0,\tag{4.3}$$

and the governing equations (3.26) and (3.27) simplify to

$$\mathrm{Div}(\partial_{\mathbf{F}}\hat{\psi}(\boldsymbol{\varepsilon}))+\mathbf{b}=\mathbf{0},\tag{4.4}$$

$$\begin{aligned}
&\mathrm{Div}(\partial_{\nabla \mathbf{F}^{\mathrm{d}}}\hat{\psi}) - (\partial_{\mathbf{F}^{\mathrm{d}}}\hat{\psi} + \partial_{\dot{\mathbf{F}}^{\mathrm{d}}}\hat{\varphi}) + \mathbf{G}^{\mathrm{d}} = \mathbf{0},\\
&\mathrm{Div}(\partial_{\nabla \mathbf{F}^{\mathrm{p}}}\hat{\psi}) - (\partial_{\mathbf{F}^{\mathrm{p}}}\hat{\psi} + \partial_{\dot{\mathbf{F}}^{\mathrm{p}}}\hat{\varphi}) + \mathbf{G}^{\mathrm{p}} = \mathbf{0},\\
&\mathrm{Div}(\partial_{\nabla \xi^{\mathrm{p}}}\hat{\psi}) - (\partial_{\xi^{\mathrm{p}}}\hat{\psi} + \partial_{\dot{\xi}^{\mathrm{p}}}\hat{\varphi}) + \mathbf{g}^{\mathrm{p}} = \mathbf{0}
\end{aligned} \tag{4.5}$$

with the potentials $\hat{\psi}$ and $\hat{\varphi}$ according to (4.2).

Eqs. (4.4) and (4.5) represent a system of coupled partial differential equations to analyse the deformation in the physical space and defect, plastic and hardening evolution in the material space. Since the gradient terms of damage, plastic and hardening evolution are included, they constitute a weakly-nonlocal theory of gradient damage coupled to gradient plasticity.

4.2. Isotropic gradient theories of damage and elastoplasticity

4.2.1. Isotropic gradient damage coupled to local finite elastoplasticity with local isotropic hardening

In the case of isotropic damage the damage tensor $\mathbf{F}^{\mathrm{d}}$ is reduced to a scalar-valued function $D(\mathbf{X}, t)$ with $0 \leqslant D \leqslant 1$,

$$\mathbf{F}^{\mathrm{d}}(\mathbf{X}, t) = D(\mathbf{X}, t)\mathbf{1}, \tag{4.6}$$

where $\mathbf{1}$ is the unit tensor. For local finite elastoplasticity with local isotropic hardening we have

$$\nabla \mathbf{F}^{\mathrm{p}} = \mathbf{0}, \quad \nabla \xi^{\mathrm{p}} = \mathbf{0}, \tag{4.7}$$

where ξ^{p} is a scalar-valued function. In this case the free energy and the dissipation pseudo-potential take the forms

$$\psi = \hat{\psi}(\mathbf{F}, D, \mathbf{F}^{\mathrm{p}}, \xi^{\mathrm{p}}, \nabla D), \quad \varphi = \hat{\varphi}(\mathbf{F}, D, \mathbf{F}^{\mathrm{p}}, \xi^{\mathrm{p}}, \nabla D, \dot{D}, \dot{\mathbf{F}}^{\mathrm{p}}, \dot{\xi}^{\mathrm{p}}), \tag{4.8}$$

and the set of material force balances (4.5) reduce to

$$\begin{aligned}
&\mathrm{Div}\left(\partial_{\nabla D}\hat{\psi}\right) - \left(\partial_{D}\hat{\psi} + \partial_{\dot{D}}\hat{\varphi}\right) + G^{\mathrm{d}} = 0,\\
&-\left(\partial_{\mathbf{F}^{\mathrm{p}}}\hat{\psi} + \partial_{\dot{\mathbf{F}}^{\mathrm{p}}}\hat{\varphi}\right) + \mathbf{G}^{\mathrm{p}} = \mathbf{0},\\
&-\left(\partial_{\xi^{\mathrm{p}}}\hat{\psi} + \partial_{\dot{\xi}^{\mathrm{p}}}\hat{\varphi}\right) + g^{\mathrm{p}} = 0.
\end{aligned} \tag{4.9}$$

The physical force balance (4.4) and the material force balances (4.9) represent the governing equations of isotropic gradient damage coupled to local finite elastoplasticity with local isotropic hardening. Here, (4.4) is a vector-valued, $(4.9)_1$ a scalar-valued, $(4.9)_2$ a tensor-valued and $(4.9)_3$ a scalar-valued equation. They are all independent balance laws coupled only by the constitutive equations (4.8). Eqs. (4.4) and $(4.9)_1$ are partial differential equations and Eqs. $(4.9)_2$ and $(4.9)_3$ represent evolution laws to determine the plastic deformation $\mathbf{F}^{\mathrm{p}}$ and the isotropic hardening parameter ξ^{p}. They are derived from local material force balance laws together with the constitutive assumptions (4.8).

The local balance law of material forces acting on dislocations $(4.9)_2$ is the basic postulate of Cermelli et al. (2001) to derive a local, thermodynamically consistent model of finite elastoplasticity to determine uniquely the nine components of $\dot{\mathbf{F}}^{\mathrm{p}}$ and also the nine components of $\mathbf{F}^{\mathrm{p}}$. While throughout the present paper we use a Lagrangian description with the physical deformation gradient $\mathbf{F}$ and the material plastic deformation measure $\mathbf{F}^{\mathrm{p}}$ as independent kinematical variables, Cermelli et al. (2001) formulate their theory in the elastic and plastic deformation gradients, $\{\mathbf{F}^{\mathrm{e}}, \mathbf{F}^{\mathrm{p}}\}$, correlated with $\{\mathbf{F}, \mathbf{F}^{\mathrm{p}}\}$ through the Bilby–Kröner–Le decomposition

$$\mathbf{F} = \mathbf{F}^{\mathrm{e}}\mathbf{F}^{\mathrm{p}}, \quad \mathbf{F}^{\mathrm{e}} \equiv \mathbf{F}\mathbf{F}^{\mathrm{p}-1}. \tag{4.10}$$

An essential simplification of the isotropic gradient damage theory coupled to local finite elastoplasticity with local isotropic hardening, as given by (4.4) and (4.9), can be obtained by assuming that elastic and plastic strains and rotations are small. Then (4.10) leads to an additive split of elastic and plastic strains

$$\mathbf{E} = \mathbf{E}^{\mathrm{e}} + \mathbf{E}^{\mathrm{p}}, \quad \mathbf{E}^{\mathrm{e}} \equiv \mathbf{E} - \mathbf{E}^{\mathrm{p}} \tag{4.11}$$

and the evolution law $(4.9)_2$ reduces to an evolution law for plastic strains leaving the plastic rotation $\mathbf{R}^{\mathrm{p}}$ undetermined.

With the small strain assumption and the additive split (4.11) the constitutive equation (4.8) can be obtained as

$$\psi = \hat{\psi}(\mathbf{E}^{\mathrm{e}}, D, \nabla D, \xi^{\mathrm{p}}), \quad \varphi = \hat{\varphi}(\mathbf{E}^{\mathrm{e}}, D, \nabla D, \xi^{\mathrm{p}}, \dot{D}, \dot{\mathbf{E}}^{\mathrm{p}}, \dot{\xi}^{\mathrm{p}}). \tag{4.12}$$

A simple assumption for the free energy $(4.12)_1$ is the following decomposition:

$$\psi = \hat{\psi}(\mathbf{E}^{\mathrm{e}}, D, \nabla D, \xi^{\mathrm{p}}) = \hat{\psi}^{\mathrm{d}}(\mathbf{E}^{\mathrm{e}}, D) + \hat{\psi}^{\nabla D}(\nabla D) + \hat{\psi}^{\mathrm{p}}(\xi^{\mathrm{p}}), \tag{4.13}$$

where we can assume

$$\hat{\psi}^{\mathrm{d}}(\mathbf{E}^{\mathrm{e}}, D) = (1 - D)\psi_0(\mathbf{E}^{\mathrm{e}}) \tag{4.14}$$

with $\psi_0(\mathbf{E}^{\mathrm{e}})$ the elastic energy of the undamaged state,

$$\psi_0(\mathbf{E}^{\mathrm{e}}) = \frac{1}{2}\left(2\mu \operatorname{tr}(\mathbf{E}^{\mathrm{e}2}) + \lambda(\operatorname{tr}\mathbf{E}^{\mathrm{e}})^2\right), \tag{4.15}$$

with μ and λ the classical Lamé coefficients, which can be expressed in terms of Young's modulus E and Poisson's ration v.

The second term on the right side of (4.13) is assumed in the simple quadratic form

$$\psi^{\nabla D} = \hat{\psi}^{\nabla D}(\nabla D) = \frac{1}{2} k \nabla D \bullet \nabla D \tag{4.16}$$

with the material parameter k to be determined by experiments (Frémond and Nedjar, 1996). In the case of strain hardening the hardening parameter ξ^{p} is not an independent function and is usually expressed by the plastic equivalent strain $\boldsymbol{\varepsilon}^{\mathrm{p}}$ with $\boldsymbol{\varepsilon}^{\mathrm{p}} \geqslant 0$, what allows us to write $\hat{\psi}^{\mathrm{p}}$ in (4.13) as

$$\hat{\psi}^{\mathrm{p}} = \hat{\psi}^{\mathrm{p}}(\xi^{\mathrm{p}}) = \hat{\psi}(\boldsymbol{\varepsilon}^{\mathrm{p}}) = \frac{h}{2}\boldsymbol{\varepsilon}^{\mathrm{p}2}, \tag{4.17}$$

where h is the plastic modulus. For perfect plasticity we have $\xi^{\mathrm{p}} = 0$ and $h = 0$.

Assuming that the dissipation pseudo-potential $(4.12)_2$ is independent of ∇D, it follows:

$$\varphi = \hat{\varphi}(\mathbf{E}^{\mathrm{e}}, D, \xi^{\mathrm{p}}, \dot{D}, \dot{\mathbf{E}}^{\mathrm{p}}, \dot{\xi}^{\mathrm{p}}) \tag{4.18}$$

with the constraint $\dot{D} \geqslant 0$.

To decouple the damage evolution from the plastic evolution, we decompose (4.18) into a damage part and a plastic part

$$\varphi = \hat{\varphi}^{\mathrm{d}}(\mathbf{E}^{\mathrm{e}}, D, \xi^{\mathrm{p}}, \dot{D}) + \hat{\varphi}^{\mathrm{p}}(D, \xi^{\mathrm{p}}, \dot{\mathbf{E}}^{\mathrm{p}}, \dot{\xi}^{\mathrm{p}}), \tag{4.19}$$

where in the case of perfect plasticity, $\xi^{\mathrm{p}} = \dot{\xi}^{\mathrm{p}} = 0$, Eq. (4.19) simplifies to

$$\varphi = \hat{\varphi}^{\mathrm{d}}(\mathbf{E}^{\mathrm{e}}, D, \dot{D}) + \hat{\varphi}^{\mathrm{p}}(D, \dot{\mathbf{E}}^{\mathrm{p}}). \tag{4.20}$$

We assume the dissipation pseudo-potential for isotropic damage and perfect plasticity in the specific form (see also Nedjar, 2001)

$$\varphi^{\mathrm{d}} = \hat{\varphi}^{\mathrm{d}}(\mathbf{E}^{\mathrm{e}}, D, \dot{D}) = \dot{D}\big(f^{\mathrm{d}} + \psi_0(\mathbf{E}^{\mathrm{e}}) - (1-D)^n \psi_0(\mathbf{E}^{\mathrm{e}+})\big) + \frac{c}{2}\dot{D}^2, \tag{4.21}$$

$$\varphi^{\mathrm{p}} = \hat{\varphi}^{\mathrm{p}}(D, \dot{\mathbf{E}}^{\mathrm{p}}) = (1-D)\sqrt{\frac{2}{3}}\boldsymbol{\sigma}_p \left\| \dot{\mathbf{E}}^{\mathrm{p}} \right\| \tag{4.22}$$

with f^{d} the damage threshold value, $\psi_0(\mathbf{E}^{\mathrm{e}})$ the undamaged elastic energy (4.15), $\psi_0(\mathbf{E}^{e+})$ the undamaged elastic energy for positive part of the elastic strain tensor, n a material parameter, c a material parameter and $\boldsymbol{\sigma}_p$ the flow stress. The yield criterion corresponding to (4.22) is the classical yield function of J_2-flow perfect plasticity formulated in terms of the effective stress $\boldsymbol{\sigma}/(1-D)$,

$$f^{\mathrm{p}}(\boldsymbol{\sigma}, D) = \frac{\|\mathrm{dev}\,\boldsymbol{\sigma}\|}{1-D} - \sqrt{\frac{2}{3}}\boldsymbol{\sigma}_p \leqslant 0. \tag{4.23}$$

4.3. Theory of elastoplasticity with gradient isotropic hardening

A simplified gradient theory of elastoplasticity is obtained by taking into account only the gradient of the isotropic hardening parameter. In this case free energy and dissipation pseudo-potential are assumed in the form

$$\psi = \hat{\psi}(\mathbf{F}, \mathbf{F}^{\mathrm{p}}, \xi^{\mathrm{p}}, \nabla\xi^{\mathrm{p}}), \quad \varphi = \hat{\varphi}(\mathbf{F}, \mathbf{F}^{\mathrm{p}}, \xi^{\mathrm{p}}, \nabla\xi^{\mathrm{p}}, \dot{\mathbf{F}}^{\mathrm{p}}, \dot{\xi}^{\mathrm{p}}). \tag{4.24}$$

With (4.11) the governing Eqs. (4.4) and (4.9) lead to

$$\begin{aligned} &\mathrm{Div}\Big(\partial_{\mathbf{F}}\hat{\psi}\Big) + \mathbf{b} = \mathbf{0}, \\ &-\Big(\partial_{\mathbf{F}^{\mathrm{p}}}\hat{\psi} + \partial_{\dot{\mathbf{F}}^{\mathrm{p}}}\hat{\varphi}\Big) + \mathbf{G}^{\mathrm{p}} = \mathbf{0}, \\ &\mathrm{Div}\Big(\partial_{\nabla\xi^{\mathrm{p}}}\hat{\psi}\Big) - \Big(\partial_{\xi^{\mathrm{p}}}\hat{\psi} + \partial_{\dot{\xi}^{\mathrm{p}}}\hat{\varphi}\Big) + g^{\mathrm{p}} = 0. \end{aligned} \tag{4.25}$$

If we assume additionally that in the free energy $\hat{\psi}$ the gradient $\nabla\xi^{\mathrm{p}}$ can be neglected, then $(4.25)_3$ reduces to the scalar-valued evolution law of the material force $\zeta^{\mathrm{p}} = \partial_{\xi^{\mathrm{p}}}\hat{\psi}$,

$$\partial_{\xi^{\mathrm{p}}}\hat{\psi} + \partial_{\dot{\xi}^{\mathrm{p}}}\hat{\varphi} - g^{\mathrm{p}} = 0. \tag{4.26}$$

In the case of strain hardening the isotropic hardening parameter ξ^{p} is a function of the plastic strain $\mathbf{E}^{\mathrm{p}} = \frac{1}{2}(\mathbf{F}^{\mathrm{p}T}\mathbf{F}^{\mathrm{p}} - \mathbf{1})$ and therefore not independent. In this case (4.26) has to be replaced by the constitutive dependency $\xi^{\mathrm{p}} = \hat{\xi}^{\mathrm{p}}(\mathbf{E}^{\mathrm{p}})$. With these additional simplifications the gradient of the isotropic hardening parameter appears only in the yield condition $(3.7)_2$. A gradient-enhanced theory of this type at small strains with gradient isotropic hardening is investigated in de Borst et al. (1993) and Sluys et al. (1993).

5. Numerical example

The model of isotropic gradient damage coupled to small strain elastoplasticity as described in Section 4.2.1 is applied to simulate numerically the splitting test of a concrete cylinder under pressure loading (Fig. 1) for elastic and elastic–ideal plastic material behavior.

The material properties are: Young's modulus $E = 26{,}170$ MPa, Poisson's ration $v = 0.18$, and the other material parameters are

$$\begin{aligned} &k = 0.2\ \mathrm{MPa} \times \mathrm{mm}^2 \quad f^{\mathrm{d}} = 0.4 \times 10^{-4}\ \mathrm{MPa}, \\ &n = 2/3, \quad c = 0.001\ \mathrm{MPa} \times \mathrm{s}, \quad \boldsymbol{\sigma}^{\mathrm{p}} = 28\ \mathrm{MPa}. \end{aligned}$$

The diameter of the cylinder is $R = 0.1524$ m and the width of the strip is $d = 0.0127$ m (see Fig. 1).

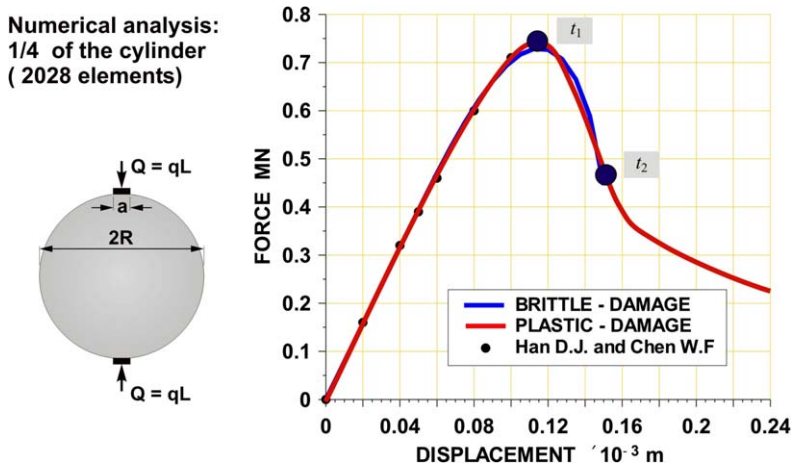

Fig. 1. Definition of the problem and deformation in the physical space.

The specimen was discretized using four-node, plane stress finite elements having at every node i two components u_i and v_i of the displacement and the damage value D_i as the nodal variables. The element matrices were calculated using 2×2 Gauss integration quadrature.

Fig. 1 shows the concrete cylinder under compression and the deformation of the cylinder in the physical space at various time instants t_i with a comparison with the results of Han and Chen (1987). In Fig. 2 the evolution of the state of damage and plastification is demonstrated for corresponding time instants t_i.

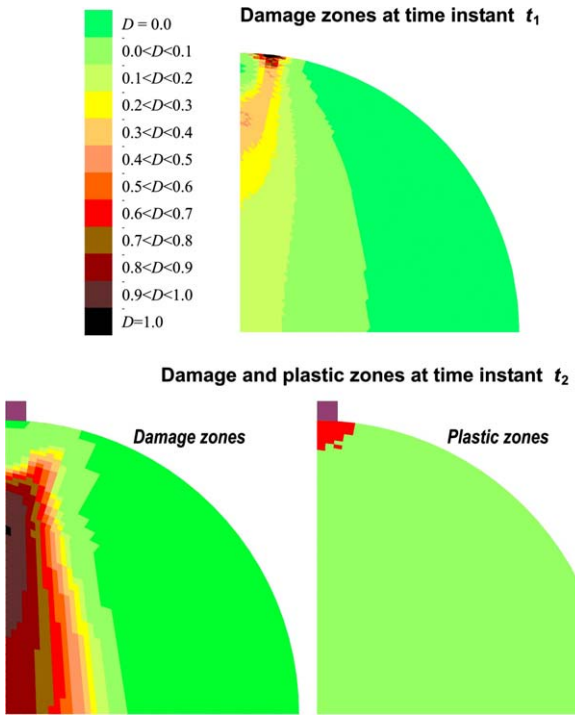

Fig. 2. Damage and plastic evolution in the material space.

6. Conclusions

The fundamental role of weakly-nonlocal (gradient-type) balance laws of material forces on microdefects and dislocations in finite elastoplasticity and damage mechanics is investigated. The balance laws of material forces together with the classical balance laws of physical forces and couples and the first and second law of thermodynamics for physical and material space together with thermodynamically admissible constitutive equations enable the analysis of dissipative deformation processes of continuous bodies with defect and plastic evolution in the material space on meso- and microlevel.

Essential features of the proposed concept are:

- Since there are as many equations as unknowns the problem is well-defined.
- Evolution laws follow from the balance laws of material forces together with the constitutive equations under the assumption that all gradient contributions can be neglected.
- Because of the weakly nonlocality of the concept the numerical analysis of localization phenomena exhibits no mesh-dependency.
- FE-discretization requires only C^0 continuity.

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References

Aifantis, E.C., 1984. On the microstructural origin of certain inelastic models. ASME J. Engng. Mat. Tech. 106, 326–330.

Bažant, Z.P., 1991. Why continuous damage is nonlocal: micromechanics arguments. Int. J. Engng. Mech. 117 (5), 1070–1087.

Bažant, Z.P., Ožbolt, J., 1990. Nonlocal microplane model for fracture, damage, and size effect in structures. J. Engng. Mech. ASCE 116, 2485–2505.

Bažant, Z.P., Pijaudier-Cabot, G., 1988. Nonlocal continuum damage, localization instability and convergence. J. Appl. Mech. 55, 287–293.

Bažant, Z.P., Planas, J., 1998. Fracture and Size Effect in Concrete and Other Quasibrittle Materials. CRC Press, Washington, DC.

Bertram, A., Kalthoff, J.F., 2003. Crack propagation toughness of rock for the range from low to very high crack speeds. Key Engineering Materials, vol. 251–252. Trans Tech Publications, Switzerland, pp. 423–430.

Cermelli, P., Fried, E., Sellers, S., 2001. Configurational stress, yield and flow in rate-independent plasticity. Proc. Roy. Soc. London A 457, 1447–1467.

Chaboche, J.L., 1988. Continuum damage mechanics: Part I: General concepts, Part II: Damage growth, crack initiation and crack growth. J. Appl. Mech. 55, 59–72.

Clayton, J.D., McDowell, D.L., Bammann, D.J., in press. Modeling dislocations and disclinations with finite micropolar elastoplasticity. Int. J. Plast.

Cleja-Tigoiu, S., 2002a. Small elastic strains in finite elastoplastic materials with continuously distributed dislocations. Theoret. Appl. Mech. 28–29, 93–112.

Cleja-Tigoiu, S., 2002b. Couple stresses and non-Riemannian plastic connection in finite elasto-plasticity. Z. Angew. Math. Phys. 53, 996–1013.

de Borst, R., 2001. Some recent issues in computational failure mechanics. Int. J. Numer. Meth. Engng. 52, 63–95.

de Borst, R., Mühlhaus, H.-B., 1992. Gradient-dependent plasticity: formulation and algorithmic aspects. Int. J. Numer. Meth. Engng. 35, 521–539.

de Borst, R., Sluys, L.J., Mühlhaus, H.-B., Pamin, J., 1993. Fundamental issues in finite element analysis of localization of deformation. Engng. Comput. 10, 99–121.

de Borst, R., Pamin, J., Peerlings, R.H.J., Sluys, L.J., 1995. On gradient-enhanced damage and plasticity models for failure in quasi-brittle and frictional materials. Comput. Mech. 17, 130–141.

Eshelby, J.D., 1951. The force on an elastic singularity. Philos. Trans. Roy. Soc. London A 224, 87–112.

Frémond, M., Nedjar, B., 1996. Damage, gradient of damage and principle of virtual power. Int. J. Solids Struct. 33, 1083–1103.

Gurtin, M.E., 2000. On the plasticity of single crystals: free energy, microforces, plastic-strain gradients. J. Mech. Phys. Solids 48 (2000), 989–1036.

Han, D.J., Chen, W.F., 1987. Constitutive modeling in analysis of concrete structures. J. Engng. Mech. 113, 577–593.

Hansen, N.R., Schreyer, H.L., 1994. A thermodynamically consistent framework for theories of elastoplasticity coupled with damage. Int. J. Solids Struct. 31 (3), 359–389.

Hirth, J.P., Lothe, J., 1982. Theory of Dislocations. Wiley and Sons.

Houlsby, G.T., Puzrin, A.M., 2000. A thermomechanical framework for constitutive models for rate-independent dissipative materials. Int. J. Plast. 16, 1017–1047.

Kachanov, L.M., 1986. Introduction to Continuum Damage Mechanics. Martinus Nijhoff Publishers, Dordrecht.

Krajcinovic, D., 1996. Damage Mechanics. Elsevier, Amsterdam.

Le, K.C., Stumpf, H., 1996a. Nonlinear continuum theory of dislocations. Int. J. Engng. Sci. 34, 339–358.

Le, K.C., Stumpf, H., 1996b. A model of elastoplastic bodies with continuously distributed dislocations. Int. J. Plast. 12, 611–627.

Le, K.C., Stumpf, H., 1996c. On the determination of the crystal reference in nonlinear continuum theory of dislocations. Proc. Roy. Soc. London A 452, 359–371.

Leibfried, G., 1949. Über die auf eine Versetzung wirkenden Kräfte. Z. Phys. 126, 781–789.

Makowski, J., Stumpf, H., 2001. Thermodynamically based concept for the modelling of continua with microstructure and evolving defects. Int. J. Solids Struct. 38, 1943–1961.

Makowski, J., Stumpf, H., Hackl, K., Triantafyllidis, T., 2004. On consistent weakly-nonlocal modeling of granular media. In: Kalpakides, Maugin (Eds.), Configurational Mechanics. Balkema Publ., Leiden–London–New York, pp. 73–86.

Miehe, C., 1998. A theoretical and computational model for isotropic elasto-plastic stress analysis in shells at large strains. Comput. Meth. Appl. Mech. Engng. 155, 193–233.

Moreau, J.J., 1970. Sur les lois de frottement, de viscosité et de plasticité. CR Acad. Sci. Paris Sér. 1 Mat. 271, 608–611.

Mosconi, M., in press. Uniqueness and minimum theorems for a multifield model of brittle solids. Int. J. Solids Struct, doi:10.1016/j.ijsolstr.2005.02.046.

Nabarro, F.R.N, 1987. Theory of Crystal Dislocations, New York.

Naghdi, P.M., Srinivasa, A.R., 1993a. A dynamical theory of structured solids. Philos. Trans. Roy. Soc. London A 345, 425–458.

Naghdi, P.M., Srinivasa, A.R., 1993b. A dynamical theory of structured solids: II. Special constitutive equations and special cases of the theory. Philos. Trans. Roy. Soc. London A, 345–459.

Nedjar, B., 2001. Elastoplastic-damage modelling including the gradient of damage: formulation and computational aspects. Int. J. Solids Struct. 38, 5421–5451.

Peach, M.O., Koehler, J.S., 1950. The forces exerted on dislocations and the stress fields produced by them. Phys. Rev. 80, 436–439.

Rakotomanana, L.R., 2004. A Geometric Approach to Thermomechanics of Dissipating ContinuaProgress in Mathematical Physics, vol. 31. Birkhäuser, Boston, Basel, Berlin.

Saczuk, J., Stumpf, H., Vallée, C., 2001. A continuum model accounting for defect and mass densities in solids with inelastic material behaviour. Int. J. Solids Struct. 38, 9545–9568.

Saczuk, J., Hackl, K., Stumpf, H., 2003. Rate theory of nonlocal gradient damage—gradient viscoinelasticity. Int. J. Plast. 19, 675–706.

Schieck, B., Stumpf, H., 1995. The appropriate corotational rate, exact formula for the plastic spin and constitutive model of finite elasto-plasticity. Int. J. Solids Struct. 32, 3643–3667.

Schieck, B., Smolenski, W.M., Stumpf, H., 1999. A shell finite element for large strain elastoplasticity with anisotropies—Part I: Shell theory and variational principle; Part II: Constitutive equations and numerical applications. Int. J. Solids Struct. 36, 5399–5424, 5425–5451.

Shizawa, K., Zbib, H.M., 1999. A thermodynamical theory of gradient elastoplasticity with dislocation density tensor. I: Fundamentals. Int. J. Plast. 15, 899–938.

Sluys, L.J., de Borst, R., Mühlhaus, H.B., 1993. Wave propagation, localization and dispersion in a gradient dependent medium. Int. J. Solids Struct. 30, 1153–1171.

Stumpf, H., Hackl, K., 2003. Micromechanical concept for the analysis of damage evolution in thermo-viscoelastic and quasi-brittle materials. Int. J. Solids Struct. 40, 1567–1584.

Stumpf, H., Hoppe, U., 1997. The application of tensor algebra on manifolds to nonlinear continuum mechanics—Invited Review Article. Z. Angew. Math. Mech. 77, 1–13.

Stumpf, H., Le, K.C., 1993. On a general concept for finite elastoplasticity based on a nonlinear continuum theory of dislocations. In: Khan, A.S. (Ed.), Proceedings of the 4th International Symposium on Plasticity and its Current Applications, Baltimore.

Stumpf, H., Saczuk, J., 2000. A generalized model of oriented continuum with defects. Z. Angew. Math. Mech. 80, 147–169.
Truesdell, C., Noll, W., 1965. The non-linear field theories of mechanics. In: Flügge, S. (Ed.), Handbuch Der Physik, vol. III/3. Springer-Verlag, Berlin.