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A continuum model accounting for defect and mass densities in solids with inelastic material behaviour

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Abstract

In this paper the analysis of structures with inelastic material behaviour is considered taking into account the evolution of defects and changes in mass density. The underlying kinematical concept of an oriented continuum is general enough to describe the micro- and macrobehaviour of material bodies appropriately. Based on the logical and consistent variational arguments for a Lagrangian functional the dynamic balance laws, boundary and transversality conditions, all related to the evolution of defect density and mass changes, are derived for macro- and microstresses of deformational as well as of configurational type. The adopted procedure, which formally leaves the balance laws unaltered, leads to the additional balance law for changes in defect density and additional boundary conditions for the changes in mass and defect densities. Driving forces or affinities, associated with the evolution of defect and mass densities, and a generalization of the J-integral representing the thermodynamic forces on defects are obtained. A nonlocal constitutive model accounting for changes in the defect density is presented. © 2001 Elsevier Science Ltd. All rights reserved.

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1. Introduction

The needs of engineers to analyse defected structures call for more refined material descriptions than classical concepts of continuum mechanics can offer. The classical macroconcept is based on the postulates of the global balance laws for linear and angular momentum, from which the local balance laws can be derived under appropriate smoothness assumptions. If the smoothness of some field quantities is not assured at discrete singular lines or surfaces within the material body, then appropriate jump conditions have to be introduced to complete the set of governing equations. In this way the formation of shear bands in crystal plasticity has been investigated by allowing for plane problems weak discontinuities of the plastic

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deformation field on singular lines leading to the so-called acoustic tensor (e.g. Asaro and Rice, 1977; Duszek-Perzyna and Perzyna, 1993; Dao and Asaro, 1996; Le et al., 1998). It is obvious that this method does not allow to determine the width of macroshear bands or to analyse coarse microshear bands (see e.g. Asaro and Rice, 1977).

On the other side, it is well known that in the finite element analysis of structures with strain localization the numerical results suffer from strong mesh sensitivity (see e.g. Roehl and Ramm, 1996; Miehe, 1998; Schieck et al., 1999a,b). The same is valid for structures with zones of heavily damaged material behaviour leading to softening and fracture process, respectively. To overcome these numerical problems various modifications of classical concepts of continuum mechanics have been proposed in the literature including higher-order spatial derivatives in the constitutive equations (e.g. Aifantis, 1992; de Borst and Mühlhaus, 1991, 1992; Sluys et al., 1993; Fleck and Hutchinson, 1997; Gao et al., 1999). With the higher-order derivatives a new length scale is introduced into the theory, where the classical balance laws remain formally unaltered. Therefore, in spite of the microingredients, these models can be considered as phenomenological ones and they are known as models of gradient plasticity or gradient damage theory. Essential is the fact that with the introduction of strain-gradient terms the governing equations remain elliptic in the softening regime and numerical procedures do not suffer extensive mesh sensitivity. This result can be obtained also by applying nonlocal models (e.g. Bažant, 1994).

Contrary to these phenomenological models with internal length scale there are various concepts of microcontinua characterized by additional balance laws for microstresses and microcouple stresses, respectively, which also entail internal length scales. The first model of this type was proposed by the Cosserats (1909), who introduced couple stresses into their theory additionally to the classical stresses. A more general description of a continuum with microstructure was introduced and investigated by Kondo (1952), Bilby et al. (1955), Kröner (1960) and Seeger (1961), who modelled dislocations, bearers of the plastic deformation, by using a nonRiemannian space structure. An alternative approach was presented by Green and Naghdi (1995), who equipped each material point with a finite number of directors for a more refined material description. Applying the kinematic assumption of the multiplicative decomposition of the total deformation gradient into elastic and plastic contributions first introduced by Bilby et al. (1955), Le and Stumpf (1996a,b) presented a nondissipative model of continua with continuously distributed dislocations at finite strain and a dissipative model of finite elastoplasticity with microstructure with the torsion tensor as additional microvariable. Based on the three directors concept to describe the crystal orientation, Naghdi and Srinivasa (1993) developed a micromodel of finite elastoplasticity, where the total deformation gradient is locally decomposed into the lattice distortion and a plastic contribution. Recently, the kinematic concept of Finslerian geometry has been applied by Saczuk (1996, 1997) to formulate a micromodel of continua with inelastic deformations.

A physically justified description of a progressive degradation of the mechanical properties of solids under loading histories, attributed to the accumulated damage, is the central problem of damage mechanics. The aim is to describe the bulk properties of continua with nucleation and evolution, growth and coalescence of microvoids and microcracks. Introducing the effective stress concept Kachanov (1958) was the first to develop a model of isotropic damage described by a scalar-valued damage variable. The continuous damage model of brittle materials presented by Krajcinovic and Fonseka (1981), Fonseka and Krajcinovic (1981) is a generalization of the scalar damage model. Further modifications of the scalar model are investigated e.g. by Kachanov (1986), Chaboche (1988a,b), Krajcinovic (1989) and Lemaitre (1992). Since both, the damage and plastification phenomena, can occur simultaneously several models have been proposed, e.g. by Simo and Ju (1987), Voyatzis and Kattan (1992), Hansen and Schreyer (1994) and Lubarda and Krajcinovic (1995) to form a more general damage description accounting for elastic–plastic deformations. A fibre bundle approach to an anisotropic damage analysis is presented by Fu et al. (1998), where the damage state is identified with a breakdown of the holonomicity in the continuum.

It is well known that defects as cracks and voids on the micro- and macrolevel can evolve and move to some extent independently of the surrounding mass and that this motion is caused by nonclassical forces, the so-called configurational forces. Furthermore, moving defects have their own inertia and kinetic energy and the motion of defects is dissipative. Eshelby (1951) was the first to investigate the force on an elastic singularity. During the last couple of years the determination of configurational forces on macrodefects has attracted considerable attention (cf. Stumpf and Le, 1990; Maugin and Trimarco, 1992; Maugin, 1993; Gurtin, 1995; Gurtin and Podio-Guidugli, 1998; Le et al., 1998, 1999).

There is an increasing evidence that the mechanical behaviour of materials with nonhomogeneous mass distribution, like in granular and porous materials, depends to a great extent on the relative arrangement of their microscopic constituents inside a representative volume element. This relative movement of the microconstituents is also responsible for the deformation-induced changes in the mass distribution. Since, for example, fracture can appear due to the presence of microcracks and initial voids, when the load is below a value to be significant for permanent deformation (Smith, 1979), it is necessary to include the changes in mass distribution to describe operating driving forces on defects.

Based on the concept of a continuum with microstructure, general enough to account for macro- and microphenomena and their interrelation, we present in this paper a constitutive model to analyse the evolution of defects taking into account the changes in the mass density. A main idea of this paper is largely motivated by the role played by mass phenomena in the materials exhibiting (dynamic) phase changes (localized phase transitions – see Truskinovsky (1993), Stanley (1971)), by the microstructural aspects of superplastic deformation (Padmanabhan and Davies, 1980) like grain boundary sliding, boundary migration, grain growth, mass transfer in porous media (Carbonell and Whitaker, 1984; Coussy, 1995), mechanics of soils (Klausner, 1991), by mass changes in the mechanism of brittle fracture of concrete and geological materials such as rocks (Scheidegger, 1974; Johannesson, 1997), by diffusion processes and defect motion.

In Section 2 we present the essential ideas of the kinematics of the underlying generalized oriented continuum model. In this concept, the assumption that the position of material points in the actual configuration is a position–direction dependent function leads to deformation and strain measures for macro- and micromotion depending on position and direction. Physical interpretations of the kinematical objects and various simplifications of the oriented continuum model are discussed.

In Section 3 we investigate a variational formulation for the continuum model accounting for the evolution of defect and mass densities. General balance laws, which do not depend on any particular material, display the strict correlation with changes in mass and defect density. Simplifications leading to the variational identity are introduced and various correlations with results of hydrodynamics and phase transition are outlined. The movable boundary (transversality) conditions written in terms of changes of defect density are reduced to an inequality widely used in fracture mechanics.

In Section 4 the Clausius–Duhem inequality for the oriented continuum considered in this paper is extended to include irreversible changes induced by the defect evolution.

In Section 5, using the Helmholtz free energy functional, the dissipation potential and the evolution equations for microstrain tensor and defect density, the rate-dependent constitutive equations accounting for the changes in defect density and a nonlocal constitutive damage model of Kachanov's type are derived.

2. Basic kinematic equations of a generalized oriented continuum model

In order to describe the heterogeneous nature of stressed (distorted) states of the body appropriately and taking into account that the motion of material particles (extended objects) is influenced by dislocations, microcracks, voids and other defects, a multidimensional configuration space with manifold structure is required.

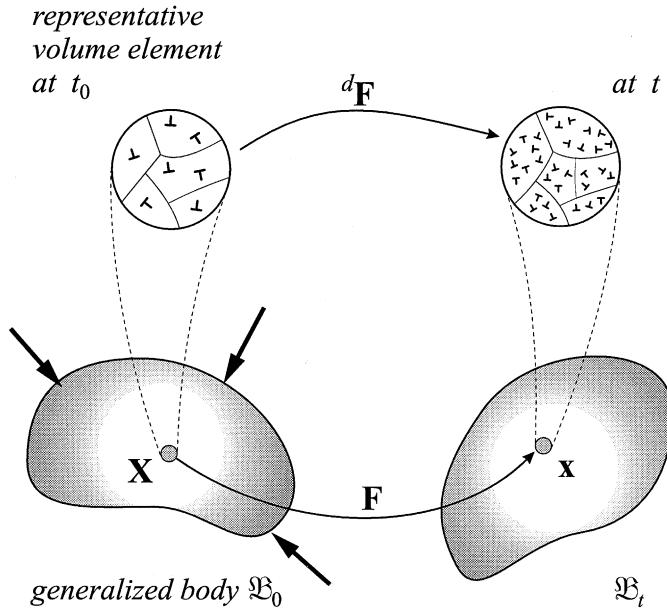


Fig. 1. Deformation of the body with structured material points within the concept of generalized oriented continuum \mathfrak{B} .

This approach means that whichever ‘internal structure’ of the body we are considering its relevant geometric properties can be modelled by a point on an appropriate manifold. A strict correlation of this approach with the nonlocal concept (Jirásek, 1998) is evident, when we replace a specific (macro) variable by its nonlocal counterpart. This can be easily shown by comparing e.g. the results of classical elasticity with those of an elastic continuum taking into account dislocations. In this case, the strain measure tensor is assumed to be composed of the classical local part (induced by the deformation gradient) and a nonlocal part according to the distribution of dislocations (cf. Teodosiu (1982), Section 18). By analogy with the idea of a nonlocal continuum, originally introduced in elasticity by Eringen (1966), a nonlocal counterpart of the oriented continuum (Stumpf and Saczuk, 2000) can be obtained by integrating the microstrain measure over the internal state space of the body under consideration. Thus, instead of using “averaging” objects defined on the three-dimensional configuration space we enlarge, according to the physical requirements, the underlying space and use a greater number of ‘local’ variables.

Within the methodology presented below points of the oriented continuum are embedded in the solid, which contains heterogeneously distributed dislocations and voids (crack dislocation arrays). In this heterogeneous medium classical particles can be viewed as individual continua (Fig. 1). We assume that any material particle (extended object), being in equilibrium, has well-defined displacements, temperature and other thermodynamics quantities within a representative volume element.

2.1. The manifold-theoretic setting

We consider a material body \mathfrak{B} with defects¹ at the equilibrium configuration C_0 , in which the density ρ_0 and the temperature θ_0 have uniform values, the stress state is not uniform and the heat flux is everywhere

¹ The bundle over the three-dimensional body (the base space) B , whose fibre at each point of B is a three-dimensional internal state space M .

zero. We will refer to C_0 as a global reference configuration and denote by C_t the configuration attained by \mathfrak{B} at the current time t . The body \mathfrak{B} is considered to be modelled by a generalized oriented continuum with material particles identified by their position \mathbf{X} (macrovector field) and direction \mathbf{D} (microvector field), briefly denoted by the pair (position, direction) = (\mathbf{X}, \mathbf{D}) in the reference configuration C_0 .

The kinematical concept to be presented in this section has to be general enough to model the fine structure of inelastic material with evolving defects at the micro- and macrolevel. It is well known that dislocations, the bearers of plastic deformation, and other defects can be modelled by using a nonEuclidean space structure with torsion (cf. Le and Stumpf, 1996a,b). On the other side, an analogous description, but of less generality, can be obtained by using an Euclidean space structure and by introducing higher order gradients, e.g. the tensor field $(\nabla \mathbf{F}^p)_{\text{skew}}$ in the model of Naghdi and Srinivasa (1993).

We assume that a deformation of the body \mathfrak{B} can be expressed in terms of the position-director-dependent deformation vector χ relating particles in the actual configuration C_t by means of a smooth invertible map

$$\mathbf{x} = \chi(\mathbf{X}, \mathbf{D}), \quad \chi : \mathfrak{B} \times \rightarrow \mathbb{E}^3 \times \mathbb{E}^3 \quad (2.1)$$

in terms of oriented particles in the reference configuration C_0 . In the manifold-theoretic setting we shall therefore consider a vector field χ on \mathfrak{B} which can give rise to a vector field $\bar{\chi}$ on the base space B . The notion of deformation is here identified with an injection χ of \mathfrak{B} into $\mathbb{E}^3 \times \mathbb{E}^3$.

We assume that the internal state of the body can be defined by specifying, for example, the material (dislocation) functional $W(\mathbf{x}, \mathbf{y})$ describing the generation and evolution of dislocations (cf. Nabarro, 1967; Hirth and Lothe, 1992; Stumpf and Saczuk, 2000). Accordingly, since cracks are responsible for the fracture of materials in a wide range of deformations (cf. Smith, 1979), the restriction of W to the dislocation functional is not a severe limitation. This convex energy functional can represent an anharmonic approximation of interactions between dislocations and their self-energy. One has to emphasize also that W is strongly dependent on a length scale of the mechanism governing the deformation at the microlevel and its morphological structure of a mesoscale volume element.

Using W we specify the nonlinear connection $\mathbf{N}_\Gamma(N_L^K)$ on \mathfrak{B} (a distribution of local tangent spaces to the distorted body \mathfrak{B}) and define the adapted nonholonomic field of frames ²

$$(\mathcal{G}_K = \mathbf{G}_K - N_K^{Ld} \mathbf{G}_L, {}^d\mathbf{G}_K)$$

with

$$\mathbf{G}_K = \frac{\partial}{\partial X^K}, \quad {}^d\mathbf{G}_K = \frac{\partial}{\partial D^K}$$

and coframes

$$(\mathbf{G}^K, {}^d\mathcal{G}^K = {}^d\mathbf{G}^K + N_L^K {}^d\mathbf{G}^L)$$

with

$$\mathbf{G}^K = dX^K, \quad {}^d\mathbf{G}^K = dD^K$$

on \mathfrak{B} . The field of frames $(\mathcal{G}_K, {}^d\mathbf{G}_K)$, in turn, is adapted to the decomposition of the tangent space

$$T\mathfrak{B} = {}^x(T\mathfrak{B}) \oplus {}^d(T\mathfrak{B})$$

² This construction is strictly correlated with the fact that there is no distinguished sub-bundle of $T\mathfrak{B}$ which complements the microbundle (vertical, in mathematical terminology) ${}^d(T\mathfrak{B})$ – see Stumpf and Saczuk (2000) and the text for further explanation.

into the sub-bundle ${}^x(T\mathfrak{B})$ spanned by \mathcal{G}_K and the sub-bundle ${}^d(T\mathfrak{B})$ spanned by ${}^d\mathbf{G}_K$ to model the macrobehaviour and the microbehaviour of the oriented material particles. In dual terms, the cotangent space

$$T^{\star}\mathfrak{B} = {}^x(T^{\star}\mathfrak{B}) \oplus {}^d(T^{\star}\mathfrak{B})$$

is decomposed correspondingly into macro- and microcotangent sub-manifolds (sub-spaces) ${}^x(T^{\star}\mathfrak{B})$ and ${}^d(T^{\star}\mathfrak{B})$ each of dimension 3, $\dim {}^x(T^{\star}\mathfrak{B}) = \dim {}^d(T^{\star}\mathfrak{B}) = 3$. The introduced sub-manifolds are, in general, spaces with torsion and curvature. According to the above decomposition of $T\mathfrak{B}$ (or $T^{\star}\mathfrak{B}$) every vector field \mathbf{Z} on \mathfrak{B} can be uniquely decomposed

$$\mathbf{Z} = {}^x\mathbf{Z} + {}^d\mathbf{Z} \quad (2.2)$$

such that ${}^x\mathbf{Z} \in {}^x(T\mathfrak{B})$ and ${}^d\mathbf{Z} \in {}^d(T\mathfrak{B})$, where ${}^x\mathbf{Z}$ is called the macropart and ${}^d\mathbf{Z}$ the micropart of \mathbf{Z} . One should note that the relation (2.2) is defined in every point $P \in \mathfrak{B}$ for ${}^x\mathbf{Z}|_P \in {}^x(T\mathfrak{B})_P = {}^x(T_P\mathfrak{B})$ and ${}^d\mathbf{Z}|_P \in {}^d(T\mathfrak{B})_P = {}^d(T_P\mathfrak{B})$.

To define covariant operators on \mathfrak{B} we proceed as follows: Assume that ∇ is a linear connection on \mathfrak{B} . The macrocovariant derivative ${}^x\nabla$ and the microcovariant derivative ${}^d\nabla$ of ∇ are defined by

$${}^x\nabla_x \mathbf{Y} = \nabla_x {}^x\mathbf{Y}, \quad {}^d\nabla_x \mathbf{Y} = \nabla_x {}^d\mathbf{Y} \quad (2.3)$$

in the algebra of Finslerian tensor fields on \mathfrak{B} .

Then covariant operators ${}^x\nabla$ and ${}^d\nabla$ for the macro- and microparts ${}^x(T\mathfrak{B})$, ${}^d(T\mathfrak{B})$ of the tangent space $T\mathfrak{B}$ are defined by

$${}^x\nabla_{\mathcal{G}_I} \mathcal{G}_J = {}^x\Gamma_{IJ}^K \mathcal{G}_K \quad (2.4)$$

and

$${}^d\nabla_{d\mathbf{G}_I} {}^d\mathbf{G}_J = {}^d\Gamma_{IJ}^K {}^d\mathbf{G}_K, \quad (2.5)$$

where coefficients ${}^x\Gamma_{IJ}^K$ of the macroconnection ${}^x\Gamma$ for the sub-bundle ${}^x(T\mathfrak{B})$ and ${}^d\Gamma_{IJ}^K$ of the microconnection ${}^d\Gamma$ for the sub-bundle ${}^d(T\mathfrak{B})$ are represented by the generalized Christoffel symbols

$${}^x\Gamma_{JK}^I = \frac{1}{2} {}^dG^{IL} (\delta_J {}^dG_{LK} + \delta_K {}^dG_{JL} - \delta_L {}^dG_{JK}), \quad (2.6)$$

$${}^d\Gamma_{JK}^I = \frac{1}{2} {}^dG^{IL} (\bar{\delta}_J {}^dG_{LK} + \bar{\delta}_K {}^dG_{JL} - \bar{\delta}_L {}^dG_{JK}). \quad (2.7)$$

The Christoffel symbols embody the relations between the holonomic distribution of the natural frames and the metric properties of the underlying space.

The connection coefficients ${}^x\Gamma_{JK}^I$ and ${}^d\Gamma_{JK}^I$ are defined in the adapted basis of ${}^x(T\mathfrak{B})$ and ${}^d(T\mathfrak{B})$, respectively. The differentiation operator δ_K used in Eq. (2.6) stands for $\delta_K = \bar{\delta}_K - N_K^L \bar{\delta}_L$, where $\bar{\delta}_K = \partial/\partial X^K$ and $\bar{\delta}_K = \partial/\partial D^K$. The introduced connection coefficients ${}^x\Gamma_{JK}^I$, ${}^d\Gamma_{JK}^I$ and N_K^L are calculated from the assumed dislocation-(microstructure-dependent) functional $W = W(\mathbf{X}, \mathbf{D})$ in terms of the metric tensor

$${}^dG_{IJ}(\mathbf{X}, \mathbf{D}) = \frac{1}{2} \bar{\delta}_I \bar{\delta}_J W(\mathbf{X}, \mathbf{D}), \quad W(\mathbf{X}, \mathbf{D}) = {}^dG_{IJ}(\mathbf{X}, \mathbf{D}) D^I D^J \quad (2.8)$$

and using the geodesic equations (the first-order evolution equations for the internal state vector \mathbf{D}) (cf. Miron, 1997)

$$\frac{dD^L}{dt} + 2G^L(\mathbf{X}, \mathbf{D}) = 0, \quad (2.9)$$

where the components of the contravariant vector G^L are given by

$$2G^L(\mathbf{X}, \mathbf{D}) = \frac{1}{2} {}^dG^{IJ} \left(\frac{\partial^2 W}{\partial D^I \partial X^K} D^K - \frac{\partial W}{\partial X^I} \right). \quad (2.10)$$

The physical meaning of the vector G^L , known as spray in the mathematical literature (Miron, 1997), will be obvious, if e.g. we assume that $D^I = \dot{X}^I$, with a dot representing the time derivative. In this case the Eq. (2.9) reduces to the second Newton's law and hence, the components G^L can be identified with appropriate (contravariant) force components (divided by two). In general, it is a curvature vector of the distribution \mathbf{N}_F .

The specified components of ${}^dG_{IJ}$ are adapted to define the metric tensor \mathbf{G} on \mathfrak{B} in the following way,

$$\mathbf{G}(\mathbf{X}, \mathbf{D}) = {}^x\mathbf{G}(\mathbf{X}, \mathbf{D}) + {}^d\mathbf{G}(\mathbf{X}, \mathbf{D}), \quad (2.11)$$

where

$$({}^x\mathbf{G}(\mathbf{X}, \mathbf{D}))_{IJ} = {}^dG_{IJ}(\mathbf{X}, \mathbf{D}) \quad \text{and} \quad ({}^d\mathbf{G}(\mathbf{X}, \mathbf{D}))_{IJ} = {}^dG_{IJ}(\mathbf{X}, \mathbf{D}).$$

Here ${}^x\mathbf{G}$ is the metric of ${}^x(T\mathfrak{B})$ and ${}^d\mathbf{G}$ the metric of ${}^d(T\mathfrak{B})$. Using the differentiation operator δ_K the macro- and microconnection coefficients (2.6) and (2.7) are finally reduced to (cf. Rund, 1959; Matsumoto, 1986)

$${}^x\Gamma_{IJK}(\mathbf{X}, \mathbf{D}) = \gamma_{IJK} - {}^d\Gamma_{KJL}N_I^L - {}^d\Gamma_{JIL}N_K^L + {}^d\Gamma_{IKL}N_J^L, \quad {}^x\Gamma_{IJK} = {}^dG_{JL}\gamma_{IK}^L, \quad (2.12)$$

where components of the Riemannian connection γ in the natural basis of ${}^x(T\mathfrak{B})$ are given by

$$\gamma_{IJK}(\mathbf{X}, \mathbf{D}) = \frac{1}{2}(\partial_K {}^dG_{IJ} + \partial_I {}^dG_{JK} - \partial_J {}^dG_{KI}), \quad \gamma_{IJK} = {}^dG_{JL}\gamma_{IK}^L \quad (2.13)$$

and the microconnection coefficients of ${}^d\Gamma$ by

$${}^d\Gamma_{IJK} = {}^dG_{JL}{}^d\Gamma_{IK}^L, \quad {}^d\Gamma_{IJK}(\mathbf{X}, \mathbf{D}) = \frac{1}{2}\bar{\partial}_K {}^dG_{IJ}(\mathbf{X}, \mathbf{D}). \quad (2.14)$$

The curvature vector of the nonlinear connection (2.10) written in terms of the coefficients γ_{JK}^I of γ and ${}^x\Gamma_{JK}^I$ of ${}^x\Gamma$ has the form

$$G^L(\mathbf{X}, \mathbf{D}) = \frac{1}{2}\gamma_{JK}^L D^J D^K, \quad N_K^L(\mathbf{X}, \mathbf{D}) = \bar{\partial}_K G^L = {}^x\Gamma_{JK}^L D^J. \quad (2.15)$$

According to Eq. (2.3) the deformation gradient \mathcal{F} of the generalized deformation χ , relative to the reference configuration C_0 , is given by

$$\mathcal{F} \equiv \nabla \chi = {}^x\mathcal{F} + {}^d\mathcal{F}, \quad (2.16)$$

with the macro- and microdeformation maps

$$\begin{aligned} {}^x\mathcal{F} &= {}^x(\nabla \chi) = {}^x\nabla \chi = \underline{\nabla \chi} = \underline{\mathbf{F}}, \\ {}^d\mathcal{F} &= {}^d(\nabla \chi) = \underline{{}^d\nabla \chi} = \underline{{}^d\mathbf{F}}. \end{aligned} \quad (2.17)$$

We assume that $\det \mathcal{F} \neq 0$.

The underlined denotations will be used in this paper. Depending on the problem under consideration the deformation gradient \mathbf{F} represents the macro- or total deformation gradient, and ${}^d\mathbf{F}$ is the micro- or inelastic deformation gradient, respectively.

In terms of the covariant derivatives (2.4) and (2.5) the deformation gradient $\mathcal{F}: T\mathfrak{B}_0 \rightarrow T\mathfrak{B}_t$ (\mathfrak{B}_0 is here identified with \mathfrak{B} at the reference time $t = 0$ and \mathfrak{B}_t with \mathfrak{B} at the current time t) in the generalized oriented continuum \mathfrak{B} is defined by the additive decomposition

$$\mathcal{F} = (\nabla + {}^d\nabla)\chi = \mathbf{F} + {}^d\mathbf{F}, \quad (2.18)$$

where the macropart $\mathbf{F}: T\mathfrak{B}_0 \rightarrow {}^x(T\mathfrak{B})$ is expressed by

$$\mathbf{F} = \nabla_{\mathcal{G}_K} \chi \otimes \mathbf{G}^K = (\mathbf{F})_K^i \mathbf{g}_i \otimes \mathbf{G}^K = \frac{\partial \chi}{\partial \mathbf{X}} - \mathbf{N}_F \frac{\partial \chi}{\partial \mathbf{D}} + {}^x\Gamma \chi, \quad (2.19)$$

the micropart ${}^d\mathbf{F}: T\mathfrak{B}_0 \rightarrow {}^d(T\mathfrak{B})$ by

$${}^d\mathbf{F} = {}^d\nabla_{\mathcal{G}_K} \chi \otimes {}^d\mathcal{G}^K = ({}^d\mathbf{F})_K^i {}^d\mathbf{g}_i \otimes {}^d\mathcal{G}^K = \frac{\partial \chi}{\partial \mathbf{D}} + {}^d\Gamma \chi \quad (2.20)$$

and the deformation function χ is given by Eq. (2.1). The base vectors in the current configuration C_t are defined by

$$\mathbf{g}_i = \frac{\partial}{\partial x^i}, \quad \mathbf{g}_i = \mathbf{g}_i - N_i^{kd} \mathbf{g}_k, \quad \mathbf{g}^i = dx^i,$$

$${}^d\mathbf{g}_i = \frac{\partial}{\partial d^i}, \quad {}^d\mathbf{g}^i = dd^i, \quad {}^d\mathbf{g}^i = {}^d\mathbf{g}^i + N_j^i \mathbf{g}^j$$

with $N_k^i = \delta_i^j \delta_k^L (N_k^L \circ \chi^{-1})$. In the component representation, Eqs. (2.19) and (2.20) take the form

$$(\mathbf{F})_K^i = \bar{\partial}_K x^i - \bar{\partial}_L x^i \bar{\partial}_K G^L + {}^x\Gamma_{IK}^i x^I, \quad (2.21)$$

$$({}^d\mathbf{F})_K^i = \bar{\partial}_K x^i + {}^d\Gamma_{IK}^i x^I \quad (2.22)$$

with

$${}^x\Gamma_{IK}^i = \delta_I^j \delta_L^L ({}^x\Gamma_{LK}^I \circ \chi^{-1}), \quad {}^d\Gamma_{IK}^i = \delta_I^j \delta_L^L ({}^d\Gamma_{LK}^I \circ \chi^{-1}).$$

There are a number of special cases allowing to simplify the representation of \mathbf{F} depending on whether (i) the internal state variables are neglected and/or (ii) \mathbf{x} is a function of \mathbf{X} or \mathbf{D} or both \mathbf{X} and \mathbf{D} . For instance, if $\mathbf{x} = \chi(\mathbf{X})$ then

$$\mathbf{F} = \frac{\partial \chi}{\partial \mathbf{X}} + \gamma \chi \quad \text{and} \quad {}^d\mathbf{F} = {}^d\Gamma \chi.$$

Note that whenever a given state of \mathfrak{B} has a nonvanishing torsion, then this state contains dislocations. This fact implies that in the case of \mathfrak{B} the objects ${}^d\Gamma_{IK}^i$ and $N_K^I = \bar{\partial}_K G^I$ are nonsingular. If the condition ${}^d\Gamma_{IK}^i = 0$ is satisfied then the micropart of deformation is Euclidean and the dissipative character of this measure is lost.

In general, the deformation gradients \mathbf{F} and ${}^d\mathbf{F}$ include the relevant (taken from the mesoscale) information on processes at the microscale, defined in the adapted, anholonomic basis. Only under severe simplifications the above deformation measures can be reduced to the classical counterparts.

With the generalized deformation gradient (Eq. (2.18), second term) a generalized Lagrangian strain tensor can be defined as

$$\mathcal{E} = \frac{1}{2}(\mathcal{C} - \mathcal{G}), \quad (2.23)$$

where

$$\mathcal{C} = \mathcal{F}^T \mathcal{F} = \mathbf{C} + {}^d\mathbf{C} \quad (2.24)$$

is a generalized right Cauchy–Green deformation tensor and the metric tensor \mathcal{G} is defined by Eq. (2.11). In turn, the macropart and micropart of the Cauchy–Green tensor \mathcal{C} are given by

$$\mathbf{C} = \mathbf{F}^T \mathbf{g} \mathbf{F}, \quad {}^d\mathbf{C} = ({}^d\mathbf{F})^T {}^d\mathbf{g} {}^d\mathbf{F}. \quad (2.25)$$

The deformation measures (2.25) being defined in an invariant manner depend crucially on the analytical form of the functional modelling the internal state of \mathfrak{B} .

2.2. Simplifications of the kinematical concept

The general concept of an oriented continuum presented in this section can be simplified by introducing restricting assumptions leading to the models of continua with microstructure known from the literature (e.g. Naghdi and Srinivasa, 1993; Le and Stumpf, 1996a,b).

Introducing the following assumptions the kinematics can be simplified as follows:

(i) The metric tensor (2.11) is a function of position only, i.e. $\mathcal{G} = \mathcal{G}(\mathbf{X})$.

In this case the potential W has the form

$$W(\mathbf{X}, \mathbf{D}) = {}^dG_{JK}(\mathbf{X})D^J D^K,$$

representing a harmonic approximation to the internal energy of dislocations. Corresponding to the second term of Eq. (2.14) the coefficients of the microconnection ${}^d\Gamma_{JK}$ are singular. It means physically that, at least locally, there are no distinguished defects. The condition

$${}^d\Gamma_{JK} = 0$$

specifies the class of all Riemannian spaces underlying the flatness of the sub-bundle ${}^d(T\mathfrak{B})$ of $T\mathfrak{B}$. Moreover, the macroconnection ${}^x\Gamma = \gamma$ and the covariant operator ${}^d\nabla_K$ is reduced to $\bar{\partial}_K$. Since the curvature vector G^L of the nonlinear connection \mathbf{N}_L is nonsingular, we have still to use the adapted field of frames $(\mathcal{G}_K, {}^d\mathbf{G}_K)$ to characterize the local geometric state of \mathfrak{B} . In this case, the definitions of \mathbf{F} and ${}^d\mathbf{F}$ retain the original meaning, while their absolute tensor representations are given by

$$\mathbf{F} = \frac{\partial \chi}{\partial \mathbf{X}} - \mathbf{N}_L \frac{\partial \chi}{\partial \mathbf{D}} + \gamma \chi \quad (2.26)$$

and

$${}^d\mathbf{F} = \frac{\partial \chi}{\partial \mathbf{D}}. \quad (2.27)$$

If we assume that the director \mathbf{D} is a function of position, $\mathbf{D} = \mathbf{D}(\mathbf{X})$, then Eq. (2.27) can be identified with the plastic distortion tensor \mathbf{F}^p (Le and Stumpf, 1996a,b; Naghdi and Srinivasa, 1993). In this case the first and third term on the right-hand side of Eq. (2.26) constitute the classical deformation gradient, while the second term responsible for the microdeformation can be identified with the macrostate through the connection (wryness) Γ induced by \mathbf{F}^p and the torsion tensor \mathbf{T}^p of this connection. In the discussed case $\Gamma = (\mathbf{F}^p)^{-1} \operatorname{grad} \mathbf{F}^p$ and $\mathbf{T}^p = \operatorname{skew}(\Gamma)$.

An identification of the material potential W with a (self and interaction) energy of dislocations at any given position of the dislocated body \mathfrak{B} and using the geometric fact that ${}^x\mathbf{T} = \operatorname{skew}(\nabla \mathbf{N}_L)$ is the torsion tensor of \mathfrak{B} at the macrolevel makes it possible to calculate the closure failure at this point. If we define a measure of this failure by

$$\mathbf{B} = - \int_S {}^x\mathbf{T} d\mathbf{S},$$

then the quantity \mathbf{B} can be interpreted as the total Burgers vectors of all dislocations cutting the surface S with the boundary ∂S . Its quantity can be identified with n dislocations multiplied by the components of the Burgers vector, where n is the number of dislocation lines cutting a unit cross-sectional area. The arguments used in deriving this result are applicable to both edge and screw dislocations.

(ii) The nonlinear connection \mathbf{N}_L vanishes.

In the case of a singular nonlinear connection, $\mathbf{N}_L = 0$, this further simplification leads to a decoupling of macro- and microbehaviour of the oriented material particle. It means that \mathfrak{B} , correspondingly the dislocated body, has locally an Euclidean space structure. As a special case of Eq. (2.1) the kinematics of \mathfrak{B} can be described then by two smooth functions (cf. Le and Stumpf, 1998)

$$\mathbf{x} = \phi(\mathbf{X}) \quad (2.28)$$

and

$$\mathbf{d} = \mathcal{D}(\mathbf{X})\mathbf{D}, \quad (2.29)$$

where $\mathbf{D} = (D^1, D^2, D^3)$ is the director in the initial and $\mathbf{d} = (d^1, d^2, d^3)$ the director in the actual configuration, and \mathcal{D} denotes a linear map³. From the geometric point of view the two functions (2.28) and (2.29) represent, in reality, coordinate transformations (extended point transformations) in $\mathbb{E}^3 \times \mathbb{E}^3$, where \mathbb{E} denotes the Euclidean space.

Moreover, the local bases \mathbf{G}_K and ${}^d\mathbf{G}_K$ have now the property of transforming as bases of \mathfrak{B} and the covariant operators (2.4) and (2.5) become Euclidean differential operators. In other words, if the decoupling of macro- and micromotion is assumed one can use the standard continuum mechanics methodology for an independent description of the body and its microstructure.

3. Variational formulation

3.1. The first-order action integral

The aim of this section is to outline the relationship between effects induced by the deformation itself and those generated by the changes in defect and mass densities and to show their influence on the physical and material strain and stress tensors.

According to the defined macro- and microdeformation gradients (2.19) and (2.20), we assume the following form of a very general functional

$$I_t = \int_G \int_T \mathcal{L}_t(\mathbf{x}; \boldsymbol{\beta}) \rho_0 \, dV \, dt, \quad (3.1)$$

where the specified arguments of \mathcal{L}_t are given by

$$\boldsymbol{\alpha} = \{\mathbf{X}, \mathbf{D}, \mathbf{x}(\mathbf{X}, \mathbf{D}, t), \mathbf{F}, {}^d\mathbf{F}, \dot{\mathbf{x}}\}, \quad \boldsymbol{\beta} = \{\rho_0(\mathbf{X}, \mathbf{D}, \mathbf{x}), d(\mathbf{X}, \mathbf{D}, \mathbf{x}), \nabla \rho_0, {}^d\nabla \rho_0, \nabla d, {}^d\nabla d\}.$$

The arguments ρ_0 and d in $\boldsymbol{\beta}$ represent, respectively, the (reference) mass density and the crack density or, more general, the defect density. The Lagrangian (deformation energy) density \mathcal{L}_t in Eq. (3.1) is assumed as a smooth map

$$\mathcal{L}_t : \mathbb{E}^6 \times J^1(\mathbb{E}^6) \rightarrow \mathbb{R}$$

with $J^1(\cdot)$ being the first jet bundle (cf. Libermann and Marle, 1986), and G denotes a fixed, closed and simply connected region in the six-dimensional space of (\mathbf{X}, \mathbf{D}) , bounded by the surface ∂G . The region G is here identified with a part of the body \mathfrak{B} . The volume element associated with any of the inelastically distorted states considered in Eq. (3.1) is defined by

$$dV = \sqrt{\mathcal{G}} \, d\mathbf{X} \, d\mathbf{D} = \sqrt{\mathcal{G}} \, dX^1 \, dX^2 \, dX^3 \, dD^1 \, dD^2 \, dD^3, \quad (3.2)$$

where \mathcal{G} is the determinant of the metric tensor \mathcal{G} according to Eq. (2.11).

The following denotations will be used throughout the next sections. The variations of vector and tensor fields defined on the macrospace ${}^x(T\mathfrak{B})$ and microspace ${}^d(T\mathfrak{B})$, respectively, will be denoted by

$$\delta \mathbf{x} = {}^x(\delta \mathbf{x}) + {}^d(\delta \mathbf{x}), \quad (3.3)$$

where

$${}^x(\delta \mathbf{x}) = \underline{{}^x\delta \mathbf{x}} = \underline{\delta \mathbf{x}}, \quad {}^d(\delta \mathbf{x}) = \underline{{}^d\delta \mathbf{x}} = \underline{\delta^d \mathbf{x}} \quad (3.4)$$

and

³ In Le and Stumpf (1998) the linear map \mathcal{D} is denoted by \mathbf{F}^e .

$$\delta\mathcal{F} = {}^x(\delta\mathcal{F}) + {}^d(\delta\mathcal{F}) \quad (3.5)$$

with the variations of the macro- and microdeformation gradients

$$\begin{aligned} {}^x(\delta\mathcal{F}) &= \delta^x\mathcal{F} = \delta^x\nabla\mathbf{x} = \delta\nabla\mathbf{x} = \underline{\delta\mathbf{F}}, \\ {}^d(\delta\mathcal{F}) &= \delta^d\mathcal{F} = \underline{\delta^d\nabla\mathbf{x}} = \underline{\delta^d\mathbf{F}}. \end{aligned} \quad (3.6)$$

For an oriented material particle with position \mathbf{X} and direction \mathbf{D} , represented by the pair (\mathbf{X}, \mathbf{D}) , its variation will be denoted by $\delta(\mathbf{X}, \mathbf{D}) = (\delta\mathbf{X}, \delta\mathbf{D})$.

For a scalar function f we need not distinguish between $\nabla_I f$ and $\delta_I f$, ${}^d\nabla_I f$ and $\bar{\delta}_I f$.

We consider now the variational derivative of the functional (3.1) given by

$$\delta I_t = \int_G \int_T (\delta\mathcal{L}_t \rho_0) dV dt + \int_G \int_T \mathcal{L}_t \rho_0 \delta(dV dt), \quad (3.7)$$

where

$$\delta(dV) = \delta(\sqrt{\mathcal{G}} d\mathbf{X} d\mathbf{D}) = [D(\delta\mathbf{X}) + {}^dD(\delta\mathbf{D})] dV \quad (3.8)$$

and

$$D(\delta\mathbf{X}) = \nabla(\delta\mathbf{X}) + \frac{\partial(\delta\mathbf{X})}{\partial\mathbf{x}} \nabla\mathbf{x}, \quad {}^dD(\delta\mathbf{D}) = {}^d\nabla(\delta\mathbf{D}) + \frac{\partial(\delta\mathbf{D})}{\partial\mathbf{x}} {}^d\nabla\mathbf{x}.$$

After using Stokes' theorem the variational derivative (3.7) can be transformed to the variational identity

$$\begin{aligned} \delta I_t &= \int_G \int_T \left[(\operatorname{div}\mathbf{T} + \mathbf{f} - \dot{\mathbf{p}}) \cdot \delta\mathbf{x} + (\operatorname{div}{}^d\mathbf{T} + {}^d\mathbf{f} - {}^d\dot{\mathbf{p}}) \cdot \delta{}^d\mathbf{x} + (\operatorname{div}\mathbb{T} + \mathbb{f} - \dot{\mathbf{p}}) \cdot \delta\mathbf{X} + (\operatorname{div}{}^d\mathbb{T} + {}^d\mathbb{f} - {}^d\dot{\mathbf{p}}) \cdot \delta\mathbf{D} \right. \\ &\quad \left. + \frac{\delta\mathcal{L}_t}{\delta d} \cdot \delta d + \frac{\delta\mathcal{L}_t}{\delta d} \cdot \delta{}^d d \right] \rho_0 dV dt - \int_{\partial G} \int_T \left(\mathbb{T}\mathbf{N} \cdot \delta\mathbf{X} + \mathbf{T}\mathbf{N} \cdot \delta\mathbf{x} + {}^d\mathbb{T}{}^d\mathbf{N} \cdot \delta\mathbf{D} + {}^d\mathbf{T}{}^d\mathbf{N} \cdot \delta{}^d\mathbf{x} \right. \\ &\quad \left. - \rho_0 \frac{\partial\mathcal{L}_t}{\partial\nabla\rho_0} \mathbf{N}\mathbf{F}^{-1} \cdot \delta\mathbf{F} - \rho_0 \frac{\partial\mathcal{L}_t}{\partial{}^d\nabla\rho_0} {}^d\mathbf{N}{}^d\mathbf{F}^{-1} \cdot \delta{}^d\mathbf{F} - \frac{\partial\mathcal{L}_t}{\partial\nabla d} \cdot \mathbf{N}\delta d - \frac{\partial\mathcal{L}_t}{\partial{}^d\nabla d} \cdot {}^d\mathbf{N}\delta{}^d d \right) \rho_0 dS dt. \end{aligned} \quad (3.9)$$

In the identity (3.9) we defined:

(a) the macro- and microstress tensors of first Piola–Kirchhoff type ⁴ by

$$\mathbf{T} = -\frac{\partial\mathcal{L}_t}{\partial\mathbf{F}} - \frac{\partial\mathcal{L}_t}{\partial\rho_0} \mathbf{F}^{-1}, \quad (3.10)$$

$${}^d\mathbf{T} = -\frac{\partial\mathcal{L}_t}{\partial{}^d\mathbf{F}} - \frac{\partial\mathcal{L}_t}{\partial\rho_0} {}^d\mathbf{F}^{-1}. \quad (3.11)$$

The additional terms $(\delta\mathcal{L}/\delta\rho_0)\mathbf{F}^{-1}$ and $(\delta\mathcal{L}/\delta\rho_0){}^d\mathbf{F}^{-1}$ are macro- and microcontributions due to changes in the mass density ρ_0 according to the assumed rule

$$\delta\rho_0 := \rho\delta\mathcal{J} = \rho_0\mathcal{F}^{-1} \cdot \delta\mathcal{F} = \rho_0(\mathbf{F}^{-1} \cdot \delta\mathbf{F} + {}^d\mathbf{F}^{-1} \cdot \delta{}^d\mathbf{F}),$$

where $\mathcal{J} = \det\mathcal{F}$.

(b) configurational macro- and microstress tensors (cf. Fried and Gurtin, 1994) by

$$\mathbb{T} = \mathbb{T}_f + \mathbb{T}_c, \quad {}^d\mathbb{T} = {}^d\mathbb{T}_f + {}^d\mathbb{T}_c,$$

⁴ The minus sign of the following formulae is correlated with the definition of the Lagrangian, $\mathcal{L}_t = K - U$, where K is the kinetic energy, while U represents the potential energy.

where the macro- and microparts \mathbb{T}_f and ${}^d\mathbb{T}_f$ of \mathbb{T} and ${}^d\mathbb{T}$, caused by the inhomogeneities of the deformation, are given by (cf. Stumpf and Saczuk, 2000)

$$\mathbb{T}_f = -\mathcal{L}_t \mathbf{1} - \mathbf{F}^T \mathbf{T}, \quad {}^d\mathbb{T}_f = -\mathcal{L}_t {}^d\mathbf{1} - ({}^d\mathbf{F})^T {}^d\mathbf{T}. \quad (3.12)$$

The configurational macro- and microparts \mathbb{T}_c and ${}^d\mathbb{T}_c$ of \mathbb{T} and ${}^d\mathbb{T}$, due to changes in the mass and defect densities, are defined by

$$\begin{aligned} \mathbb{T}_c &= \frac{\delta \mathcal{L}_t}{\delta \rho_0} \mathbf{1} + \frac{\partial \mathcal{L}_t}{\partial \nabla \rho_0} \otimes \nabla \rho_0 + \frac{\partial \mathcal{L}_t}{\partial \nabla d} \otimes \nabla d, \\ {}^d\mathbb{T}_c &= \frac{\delta \mathcal{L}_t}{\delta \rho_0} {}^d\mathbf{1} + \frac{\partial \mathcal{L}_t}{\partial {}^d \nabla \rho_0} \otimes {}^d \nabla \rho_0 + \frac{\partial \mathcal{L}_t}{\partial {}^d \nabla d} \otimes {}^d \nabla d, \end{aligned} \quad (3.13)$$

with the affinities of ρ_0 and d given by (cf. Truskinovsky, 1993)

$$\frac{\delta \mathcal{L}_t}{\delta \rho_0} = \rho_0 \left[\frac{\partial \mathcal{L}_t}{\partial \rho_0} - \frac{1}{\rho_0} \operatorname{div} \left(\rho_0 \frac{\partial \mathcal{L}_t}{\partial \nabla \rho_0} \right) \right], \quad \frac{\delta \mathcal{L}_t}{\delta d} = -\operatorname{div} \left(\rho_0 \frac{\partial \mathcal{L}_t}{\partial {}^d \nabla \rho_0} \right),$$

$$\frac{\delta \mathcal{L}_t}{\delta d} = \frac{\partial \mathcal{L}_t}{\partial d} - \frac{1}{\rho_0} \operatorname{div} \left(\rho_0 \frac{\partial \mathcal{L}_t}{\partial \nabla d} \right), \quad \frac{\delta \mathcal{L}_t}{\delta {}^d d} = \frac{1}{\rho_0} \operatorname{div} \left(\rho_0 \frac{\partial \mathcal{L}_t}{\partial {}^d \nabla d} \right).$$

In Eq. (3.13) the symbol \otimes denotes the tensor product of vectors. A generalized derivation operator $\delta(\cdot)/\delta\alpha$ for $\alpha = \rho_0$ or d , known as the Volterra derivative (cf. Beris and Edwards, 1994) is defined as (cf. Gyarmati, 1970; Truskinovsky, 1993)

$$\frac{\delta(\cdot)}{\delta \alpha} = \frac{\partial(\cdot)}{\partial \alpha} - \operatorname{div} \left(\frac{\partial(\cdot)}{\partial \nabla \alpha} \right).$$

The above affinities can be used to model the internal dissipation, associated with the motion of defects (moving discontinuities), using the relaxation evolution equations at the macroscale⁵ (cf. Truskinovsky, 1993; Fried and Gurtin, 1994)

$$\dot{d} = -\lambda \frac{\delta \mathcal{L}_t}{\delta d} \quad (3.14)$$

and microscale

$${}^d\dot{d} = -{}^d\lambda \frac{\delta \mathcal{L}_t}{\delta {}^d d},$$

where λ and ${}^d\lambda$ are positive kinetic coefficients characterizing the time relaxations at both levels. In order to guarantee the nonnegative dissipation (in the absence of any other dissipation mechanism) the following requirement

$$\rho_0 \left(\lambda \frac{\delta \mathcal{L}_t}{\delta d} \cdot \frac{\delta \mathcal{L}_t}{\delta d} + {}^d\lambda \frac{\delta \mathcal{L}_t}{\delta {}^d d} \cdot \frac{\delta \mathcal{L}_t}{\delta {}^d d} \right) \geq 0$$

must be satisfied at each point of the defected body and at all times.

Furthermore we define:

(c) macro- and micromomentum vectors by

⁵ If we put $\mathcal{L}_t(d, \nabla d, \cdot) = \mathcal{L}_0(d, \cdot) + a(\cdot)|\nabla d|^2$ then Eq. (3.14) leads to the Ginzburg–Landau equation (Hohenberg and Halperin, 1977).

$$\mathbf{p} = \frac{\partial \mathcal{L}_t}{\partial \dot{\mathbf{x}}}, \quad {}^d\mathbf{p} = \frac{\partial \mathcal{L}_t}{\partial {}^d\dot{\mathbf{x}}}, \quad (3.15)$$

(d) configurational macro- and micromomentum vectors⁶ by

$$\mathbf{p} = \frac{\partial \mathcal{L}_t}{\partial \dot{\mathbf{X}}}, \quad {}^d\mathbf{p} = \frac{\partial \mathcal{L}_t}{\partial {}^d\dot{\mathbf{X}}}, \quad (3.16)$$

(e) external and internal body forces by

$$\mathbf{f} = \frac{\partial \mathcal{L}_t}{\partial \mathbf{x}}, \quad {}^d\mathbf{f} = \frac{\partial \mathcal{L}_t}{\partial {}^d\mathbf{x}}, \quad (3.17)$$

(f) the macro-and microinhomogeneity forces by

$$\mathbf{f} = \nabla \mathcal{L}_t, \quad {}^d\mathbf{f} = {}^d\nabla \mathcal{L}_t \quad (3.18)$$

and

(g) the generalized divergence operator div of \mathbf{T} , ${}^d\mathbf{T}$, \mathbb{T} and ${}^d\mathbb{T}$ by

$$\text{div} \mathbf{T} = D\mathbf{T} - \bar{\partial} \mathbf{G} {}^d D\mathbf{T} - \mathbf{T}^x \Gamma, \quad \text{div} {}^d\mathbf{T} = {}^d D {}^d\mathbf{T} - {}^d\mathbf{T} {}^d \Gamma,$$

$$\text{div} \mathbb{T} = -\nabla \mathcal{L}_t - \mathbf{F}^T (\mathbf{f} + \text{div} \mathbf{T}), \quad \text{div} {}^d\mathbb{T} = -{}^d\nabla \mathcal{L}_t - ({}^d\mathbf{F})^T ({}^d\mathbf{f} + \text{div} {}^d\mathbf{T}).$$

3.1.1. Remark on nonhomogeneous mass distribution

A relative motion of the microconstituents of \mathfrak{B}_t is generally responsible for the deformation-induced changes in the mass distribution. Our approach, which offers a unified description of the internal state structure of \mathfrak{B}_t , can easily be adopted to model deformation-induced changes in the mass. For example, a model of deforming double (fissured) porous medium (Khalili and Valliappan, 1996), regarded as a multiphase material (Bowen and Wiese, 1969; Ehlers and Volk, 1998) can be treated as a classical example of the presented theory. Here, by the fissured porous medium we understand two overlapping flow regions of a porous skeleton and a fissured network, both saturated with compressible fluid.

To describe averaged quantities, such as the defect density, which can be randomly distributed or with inherently localized microscopic constituents in the representative volume element, we demand that every representative volume element has at every instant a well-defined state. Taking this for granted, it is possible to assure the existence of trajectories for its evolution and to apply for its analysis the geometric setting of Section 2. It can be shown that the physical objects ${}^d\mathbf{T}$, ${}^d\mathbb{T}$, ${}^d\mathbf{f}$ and ${}^d\mathbf{f}$ can be used to model the fissured structure, the internal one for the porous skeleton of \mathfrak{B}_t , while \mathbf{T} , \mathbb{T} , \mathbf{f} and \mathbf{f} can be adopted to describe the porous skeleton of \mathfrak{B}_t . One has to emphasize that the two (porous and fissured) flow regions are coupled not only through the leakage term (like in the theory of Khalili and Valliappan (1996)), but also through the internal state of the fissured network.

The flow model of \mathfrak{B}_t , based on the double porosity concept can be obtained by combining the mass conservation, Darcy's law and an equation of state for the fluid.

All variational derivatives are obtained under the assumption that the system (the body with loads) admits a one-parameter transformation group acting on the independent and dependent variables in the form

⁶ The position and the direction in the reference configuration C_0 are here considered to be functions of time. In general, the configurational objects are indeterminate in the absence of configurational changes.

$$\begin{aligned}\bar{X}^I &= X^I + V_X^I(X^M, D^M, x^n)\epsilon + o(\epsilon), \\ \bar{D}^I &= D^I + V_D^I(X^M, D^M, x^n)\epsilon + o(\epsilon), \\ \bar{x}^i &= x^i + v_x^i(X^M, D^M, x^n)\epsilon + o(\epsilon),\end{aligned}\tag{3.19}$$

where ϵ denotes a scalar parameter, while $V_X^I(\cdot)$, $V_D^I(\cdot)$ and $v_x^i(\cdot)$ are class C^1 functions of their variables such that

$$\bar{X}^I(0) = X^I, \quad \bar{D}^I(0) = D^I, \quad \bar{x}^i(0) = x^i \tag{3.20}$$

for $\epsilon \rightarrow 0$.

In order to obtain a definite insight into the variational identity (3.9), let us consider various cases of dependent variables. In particular

Case (α): If $\mathcal{L}_t = \mathcal{L}_t(\alpha)$ with $\alpha = \{\mathbf{x}, \mathbf{F}\}$ then the relevant definitions of field variables (3.10)–(3.18) are reduced to the following ones

$$\begin{aligned}\mathbf{T} &= -\frac{\partial \mathcal{L}_t}{\partial \mathbf{F}}, \\ \mathbf{f} &= \frac{\partial \mathcal{L}_t}{\partial \mathbf{x}},\end{aligned}\tag{3.21}$$

while the variational identity (3.9) reduces to the static version

$$\delta I_t = \int_G (\operatorname{div} \mathbf{T} + \mathbf{f}) \cdot \delta \mathbf{x} \rho_0 dV - \int_{\partial G} \mathbf{T} \mathbf{N} \cdot \delta \mathbf{x} \rho_0 dS$$

of the classical variational identity.

Case (β): If $\mathcal{L}_t = \mathcal{L}_t(\alpha, \beta)$ with $\alpha = \{\mathbf{X}\}$ and $\beta = \{\rho, d, \nabla \rho, \nabla d\}$ then the relevant definitions of field variables (3.10)–(3.18) are reduced to the following ones (cf. Beris and Edwards, 1994; Truskinovsky, 1993)

$$\begin{aligned}\mathbb{T} &= \frac{\delta \mathcal{L}_t}{\delta \rho} \mathbf{1} + \frac{\delta \mathcal{L}_t}{\delta \nabla \rho} \otimes \nabla \rho + \frac{\delta \mathcal{L}_t}{\delta \nabla d} \otimes \nabla d, \\ \mathbf{f} &= \nabla \mathcal{L}_t.\end{aligned}\tag{3.22}$$

In this case the variational identity (3.9) written in the form

$$\delta I_t = \int_G \left(\operatorname{div} \mathbb{T} \cdot \delta \mathbf{X} + \frac{\delta \mathcal{L}_t}{\delta d} \cdot \delta d \right) \rho dV - \int_{\partial G} \left(\mathbb{T} \mathbf{N} \cdot \delta \mathbf{X} - \rho \frac{\delta \mathcal{L}_t}{\delta \nabla \rho} \mathbf{N} \mathbf{F}^{-1} \cdot \delta \mathbf{F} - \frac{\delta \mathcal{L}_t}{\delta \nabla d} \cdot \mathbf{N} \delta d \right) \rho dS \tag{3.23}$$

corresponds to the identity (3.3) of Truskinovsky (1993). There, this case was used to define a nonlocal gradient-type constitutive model for material inside the transition layer in a compressible fluid. Note that the term $\rho \mathbf{F}^{-1} \cdot \delta \mathbf{F}$ in the surface integral is equal to $\rho \operatorname{div} \delta \mathbf{X}$ and the parameters ξ (here d) in Truskinovsky (1993) is considered as an internal parameter characterizing the state of the material in an interface layer.

Case (γ): If $\mathcal{L}_t = \mathcal{L}_t(\alpha, \beta)$ with $\alpha = \{\mathbf{X}, \mathbf{D}, \mathbf{x}\}$ and $\beta = \{\rho_0, d, \nabla \rho_0, {}^d \nabla \rho_0, \nabla d, {}^d \nabla d\}$, the field variables (3.10)–(3.18) are obtained as

$$\begin{aligned}
\mathbf{T} &= -\frac{\delta \mathcal{L}_t}{\delta \rho_0} \mathbf{F}^{-1}, \\
{}^d \mathbf{T} &= -\frac{\delta \mathcal{L}_t}{\delta \rho_0} {}^d \mathbf{F}^{-1}, \\
\mathbb{T} &= \left(\frac{\delta \mathcal{L}_t}{\delta \rho_0} - \mathcal{L}_t \right) \mathbf{1} + \frac{\partial \mathcal{L}_t}{\partial \nabla \rho_0} \otimes \nabla \rho_0 + \frac{\partial \mathcal{L}_t}{\partial \nabla d} \otimes \nabla d, \\
{}^d \mathbb{T} &= \left(\frac{\delta \mathcal{L}_t}{\delta \rho_0} - \mathcal{L}_t \right) {}^d \mathbf{1} + \frac{\partial \mathcal{L}_t}{\partial {}^d \nabla \rho_0} \otimes {}^d \nabla \rho_0 + \frac{\partial \mathcal{L}_t}{\partial {}^d \nabla d} \otimes {}^d \nabla d, \\
\mathbf{f} &= \frac{\partial \mathcal{L}_t}{\partial \mathbf{x}}, \\
{}^d \mathbf{f} &= \frac{\partial \mathcal{L}_t}{\partial {}^d \mathbf{x}}, \\
\mathbf{f} &= \nabla \mathcal{L}_t, \\
{}^d \mathbf{f} &= {}^d \nabla \mathcal{L}_t.
\end{aligned} \tag{3.24}$$

Case (δ): If $\mathcal{L}_t = \mathcal{L}_t(\boldsymbol{\alpha}, \boldsymbol{\beta})$ with $\boldsymbol{\alpha} = \{\mathbf{X}, \mathbf{D}, \mathbf{x}, \mathbf{F}\}$ and $\boldsymbol{\beta} = \{\rho_0, \nabla \rho_0\}$, the relevant definitions of field variables (3.10)–(3.18) are reduced to

$$\begin{aligned}
\mathbf{T} &= -\frac{\partial \mathcal{L}_t}{\partial \mathbf{F}} - \frac{\delta \mathcal{L}_t}{\delta \rho_0} \mathbf{F}^{-1}, \\
\mathbb{T} &= \left(\frac{\delta \mathcal{L}_t}{\delta \rho_0} - \mathcal{L}_t \right) \mathbf{1} - \mathbf{F}^T \mathbf{T} + \frac{\partial \mathcal{L}_t}{\partial \nabla \rho_0} \otimes \nabla \rho_0, \\
\mathbf{f} &= \frac{\partial \mathcal{L}_t}{\partial \mathbf{x}}, \\
\mathbf{f} &= \nabla \mathcal{L}_t.
\end{aligned} \tag{3.25}$$

Case (ϵ): If $\mathcal{L}_t = \mathcal{L}_t(\boldsymbol{\alpha}, \boldsymbol{\beta})$ with $\boldsymbol{\alpha} = \{\mathbf{X}, \mathbf{D}, \mathbf{x}, \mathbf{F}\}$ and $\boldsymbol{\beta} = \{d, \nabla d\}$, the relevant definitions of field variables (3.10)–(3.18) lead to

$$\mathbf{T} = -\frac{\partial \mathcal{L}_t}{\partial \mathbf{F}}, \quad \mathbb{T} = -\mathcal{L}_t \mathbf{1} - \mathbf{F}^T \mathbf{T} + \frac{\partial \mathcal{L}_t}{\partial \nabla d} \otimes \nabla d, \quad \mathbf{f} = \frac{\partial \mathcal{L}_t}{\partial x}, \quad \mathbf{f} = \nabla \mathcal{L}_t. \tag{3.26}$$

The last case is investigated in detail in Fried and Gurtin (1994) for the dynamic solid–solid transition, where d is considered as an order parameter.

3.2. Balance laws, boundary and transversality conditions

In this section we derive a dissipative model of oriented continuum, which enables the analysis of engineering structures with inelastic material behaviour, evolving defects and mass changes. As starting point we consider the action integral (3.9) modified by including the contribution of prescribed boundary tractions \mathbf{t} , ${}^d \mathbf{t}$ with components in the actual configuration on each part of ∂G and given configurational boundary stresses \mathbf{t} , ${}^d \mathbf{t}$ in the material space. We assume that the action I_t associated with the motion of \mathfrak{B} satisfies the stationary condition

$$\delta I_t = - \int_{\partial G} \int_T (\mathbf{t} \cdot \delta \mathbf{x} + {}^d \mathbf{t} \cdot \delta {}^d \mathbf{x} + \mathbf{t} \cdot \delta \mathbf{X} + {}^d \mathbf{t} \cdot \delta \mathbf{D}) dS dt. \tag{3.27}$$

The dynamical balance laws and boundary conditions for deformational and configurational forces resulting from (3.9) and the stationarity condition (3.27) are the following:

(a) The balance of deformational and configurational macromomentum

$$\dot{\mathbf{p}} = \mathbf{f} + \operatorname{div} \mathbf{T}, \quad \dot{\mathbf{p}} = \mathbf{f} + \operatorname{div} \mathbb{T}, \quad (3.28)$$

where \mathbf{p} is the momentum vector, \mathbf{p} the Eshelbian momentum vector, \mathbf{T} the first Piola–Kirchhoff macrostress tensor, \mathbb{T} the Eshelbian macrostress tensor, \mathbf{f} the external macrobody force and \mathbf{f} the material macroinhomogeneity force.

In components, the first term of Eq. (3.28) takes the form

$$\dot{p}_k = f_k + \frac{\partial(\mathbf{T})_k^I}{\partial X^I} - \frac{\partial G^J}{\partial D^I} \frac{\partial(\mathbf{T})_k^I}{\partial D^J} - (\mathbf{T})_j^{Ix} \Gamma_{kl}^j. \quad (3.29)$$

After neglecting the dependence of \mathbf{F} and \mathbf{T} on the internal vector field \mathbf{D} , Eq. (3.29) leads to the classical form

$$\dot{p}_k = f_k + \frac{\partial(\mathbf{T})_k^I}{\partial X^I} - (\mathbf{T})_j^I \bar{\Gamma}_{kl}^j, \quad (3.30)$$

where $\bar{\Gamma}_{kl}^j$ are the connection coefficients defined on the three-dimensional configuration space.

In turn, the second term of Eq. (3.28) can be written in component form

$$(\dot{\mathbf{p}})_K = (\mathbf{f})_K + (\operatorname{div} \mathbb{T})_K,$$

where

$$(\operatorname{div} \mathbb{T})_K = -(\nabla \mathcal{L}_t)_K - (\mathbf{F})_K^k \left(\frac{\partial \mathcal{L}_t}{\partial x^k} + \frac{\partial(\mathbf{T})_k^L}{\partial X^L} - \frac{\partial G^J}{\partial D^L} \frac{\partial(\mathbf{T})_k^L}{\partial D^J} - (\mathbf{T})_j^{Lx} \Gamma_{kl}^j \right), \quad (3.31)$$

and the components $(\mathbf{F})_L^k$ are defined by Eq. (2.21). If we neglect the dependence of \mathbf{F} and \mathbf{T} on \mathbf{D} , then in the Euclidean representation $(\operatorname{div} \mathbb{T})_K$ reduces to the form (Maugin (1993), Chapter 4)

$$(\operatorname{div} \mathbb{T})_K = -\frac{\partial \mathcal{L}_t}{\partial X^K} - (\mathbf{F})_K^k \left(\frac{\partial \mathcal{L}_t}{\partial x^k} + \frac{\partial(\mathbf{T})_k^L}{\partial X^L} \right).$$

Here, we have to point out that in this case the position–direction-dependent connection coefficients ${}^x\Gamma_{kk}^j$ are not zero in the case of a defected body.

(b) The balance of moment of deformational and configurational macromomentum

$$\mathbf{FT}^T = \mathbf{TF}^T, \quad \mathbf{CT}^T = \mathbb{T}\mathbf{C}. \quad (3.32)$$

(c) The balance of deformational and configurational micromomentum

$${}^d\dot{\mathbf{p}} = {}^d\mathbf{f} + \operatorname{div} {}^d\mathbf{T}, \quad {}^d\dot{\mathbf{p}} = {}^d\mathbf{f} + \operatorname{div} {}^d\mathbb{T}, \quad (3.33)$$

where ${}^d\mathbf{p}$ is the micromomentum vector, ${}^d\mathbf{p}$ the Eshelbian micromomentum vector, ${}^d\mathbf{T}$ the first Piola–Kirchhoff microstress tensor, ${}^d\mathbb{T}$ the Eshelbian microstress tensor, ${}^d\mathbf{f}$ the internal microbody force and ${}^d\mathbf{f}$ the material microinhomogeneity force.

In component form, the first term of Eq. (3.33) reads

$$({}^d\dot{\mathbf{p}})_k = ({}^d\mathbf{f})_k + \frac{\partial({}^d\mathbf{T})_k^K}{\partial D^K} - ({}^d\mathbf{T})_j^{Ld} \Gamma_{kl}^j. \quad (3.34)$$

This equation, analogous to Eq. (3.30), is defined in terms of the internal vector field \mathbf{D} . The connection coefficients ${}^d\Gamma_{kl}^j$ represent here a measure of dislocation density defined by the dislocation potential W .

In component form, the second term of Eq. (3.33) reads

$$({}^d\dot{\mathbf{p}})_K = ({}^d\mathbf{f})_K + (\operatorname{div} {}^d\mathbb{T})_K,$$

where

$$(\operatorname{div}^d \mathbb{T})_K = -(^d \nabla \mathcal{L}_t)_K - (^d \mathbf{F})_K^k \left(\frac{\partial \mathcal{L}_t}{\partial x^k} + \frac{\partial (^d \mathbf{T})_k^L}{\partial D^L} - (^d \mathbf{T})_j^{Ld} \Gamma_{KL}^j \right), \quad (3.35)$$

and the components $(^d \mathbf{F})_K^k$ are given by Eq. (2.22). The momentum of configurational microforces is also defined on the internal state space in terms of \mathbf{D} and the dislocation functional $W = W(\mathbf{X}, \mathbf{D})$.

(d) The balance of moment of deformational and configurational macromomentum

$$^d \mathbf{F} (^d \mathbf{T})^T = ^d \mathbf{T} (^d \mathbf{F})^T, \quad ^d \mathbf{C} (^d \mathbb{T})^T = ^d \mathbb{T} ^d \mathbf{C}. \quad (3.36)$$

(e) The balance of macro- and microstress vectors induced by changes in the defect (crack) density

$$\frac{\delta \mathcal{L}}{\delta d} \equiv \frac{\partial \mathcal{L}_t}{\partial d} - \frac{1}{\rho_0} \operatorname{div} \left(\rho_0 \frac{\partial \mathcal{L}_t}{\partial \nabla d} \right) = 0, \quad \frac{\delta \mathcal{L}}{\delta \bar{d}} \equiv \operatorname{div} \left(\rho_0 \frac{\partial \mathcal{L}_t}{\partial ^d \nabla d} \right) = 0. \quad (3.37)$$

(f) The traction boundary conditions and the configurational traction boundary conditions

$$\mathbf{T} \mathbf{N} = \mathbf{t}, \quad ^d \mathbf{T} ^d \mathbf{N} = ^d \mathbf{t}, \quad \mathbb{T} \mathbf{N} = \mathbf{t}, \quad ^d \mathbb{T} ^d \mathbf{N} = ^d \mathbf{t}, \quad (3.38)$$

where \mathbf{N} and $^d \mathbf{N}$ are the outer normal vectors to the boundary $\partial \mathfrak{B}$ at macro- and microlevel, respectively.

(g) The macro- and microstress vector boundary conditions induced by changes in the defect density

$$\frac{\partial \mathcal{L}_t}{\partial \nabla d} \cdot \mathbf{N} = 0, \quad \frac{\partial \mathcal{L}_t}{\partial ^d \nabla d} \cdot ^d \mathbf{N} = 0. \quad (3.39)$$

(h) The boundary conditions of macro- and microstress vectors associated with changes in the referential mass density

$$\frac{\partial \mathcal{L}_t}{\partial \nabla \rho_0} \cdot \mathbf{N} \mathbf{F}^{-1} = 0, \quad \frac{\partial \mathcal{L}_t}{\partial ^d \nabla \rho_0} \cdot ^d \mathbf{N} ^d \mathbf{F}^{-1} = 0. \quad (3.40)$$

Here, we have to mention that the balance laws (3.28)–(3.36) are the dynamical generalizations of those presented by Stumpf and Saczuk (2000) taking furthermore into account the changes in the mass and defect densities (cf. definitions (3.10)–(3.13)). The additional balance laws (3.37) for macro- and microstress vectors associated with changes in the defect density are in effect functionally correlated with (3.28) and (3.33). Due to the absence of a functional dependence between ⁷ d and \mathbf{x} this effect was neglected here. One has to emphasize also that the boundary conditions (3.38) and (3.40) are not independent of each other (cf. (3.43)).

Case (ζ): Continuing the investigations of Section 3.1, let us consider here a further comparison of our results with those presented by Fried and Gurtin (1994). The balance of deformational macromomentum (Eq. (3.28), first term) and moment of deformational macromomentum ((3.32), first term) are identical with the Eq. (2.5) of Fried and Gurtin (1994). The resulting balance for configurational forces (Eq. (4.1), second term) in Fried and Gurtin (1994) is analogous to second term of Eq. (3.28) provided that:

(i) The force $\operatorname{div} \mathbb{T} = -\nabla \mathcal{L}_t - \mathbf{F}^T (\mathbf{f} + \operatorname{div} \mathbf{T})$ is identified with $\pi + \div \zeta$ of Fried and Gurtin (1994), where $\pi = -\nabla \mathcal{L}_t$ is an inhomogeneity force and ζ in $\div \zeta = -\mathbf{F}^T (\mathbf{f} + \operatorname{div} \mathbf{T})$ is the configurational tensor.

The presented comparison is, of course formal, since the balance for configurational forces in Fried and Gurtin (1994) is postulated.

(ii) Upon substitution of the Lagrangian $\mathcal{L}_t = \frac{1}{2} \rho_0 |\dot{\mathbf{p}}|^2 - \Psi$ into second term of Eq. (3.26), we arrive at

⁷ Of course, there are a number of Pfaffian-type constraints $A_i dx^i + A dd = 0$, where A_i and A are functions of \mathbf{x} alone.

$$\mathbb{T} = \left(\Psi - \frac{1}{2} \rho_0 |\dot{\mathbf{p}}|^2 \right) \mathbf{1} - \mathbf{F}^T \mathbf{T} + \frac{\partial \mathcal{L}_t}{\partial \nabla d} \otimes \nabla d,$$

the generalization of the Eshelbian tensor (4.4) in Fried and Gurtin (1994).

(i) Transversality conditions

For problems with movable boundaries, like those with evolving crack surfaces, an extremum of the action integral can occur only, when the solution curve is one of the integral curves of the Euler–Lagrange equations (3.28)–(3.37). To solve this problem the additional conditions must be obtained from the necessary condition for an extremum. These conditions called the transversality conditions establish some relations between the deformation gradients \mathbf{F} , ${}^d\mathbf{F}$, the reference mass gradients $\nabla \rho_0$, ${}^d\nabla \rho_0$, the defect gradients ∇d , ${}^d\nabla d$ and gradients of certain macro- and microsurfaces in motion. In this fact, among others, lies the importance of the transversality conditions. Any point on such evolving surface is moved according to the actual load system and the environmental conditions.

The variational identity (3.9) of the presented theory, equivalent to the transversality conditions for the functional (3.1), takes the form

$$\begin{aligned} \delta I_t = - \int_{\tilde{\Sigma}_t} \int_T \left(\mathbb{T} \mathbf{N} \cdot \delta \mathbf{X} + \mathbf{T} \mathbf{N} \cdot \delta \mathbf{x} + {}^d\mathbb{T}^d \mathbf{N} \cdot \delta \mathbf{D} + {}^d\mathbf{T}^d \mathbf{N} \cdot \delta^d \mathbf{x} - \rho_0 \frac{\partial \mathcal{L}_t}{\partial \nabla \rho_0} \mathbf{N} \mathbf{F}^{-1} \cdot \delta \mathbf{F} \right. \\ \left. - \rho_0 \frac{\partial \mathcal{L}_t}{\partial {}^d \nabla \rho_0} {}^d \mathbf{N} {}^d \mathbf{F}^{-1} \cdot \delta {}^d \mathbf{F} - \frac{\partial \mathcal{L}_t}{\partial \nabla d} \cdot \mathbf{N} \delta d - \frac{\partial \mathcal{L}_t}{\partial {}^d \nabla d} \cdot {}^d \mathbf{N} \delta^d d \right) \rho_0 dS dt, \end{aligned} \quad (3.41)$$

where $\tilde{\Sigma}_t = \Sigma_t \cup {}^d\Sigma_t$ may represent an external or internal surface of \mathfrak{B} . The above identity has been obtained as the result of demanding that the variational derivative (3.9) is equal zero for all variations $(\delta \mathbf{X}, \delta \mathbf{D}, \delta \mathbf{x}, \delta^d \mathbf{x}, \delta d, \delta^d d)$.

If the variations $\delta \mathbf{X}$, $\delta \mathbf{x}$ and $\delta \mathbf{D}$, $\delta^d \mathbf{x}$ are independent, neglecting then the effects induced by changes of d , the equations

$$\begin{aligned} \mathbf{T} \mathbf{N} = 0, \quad \mathbf{T} \mathbf{N} = \rho_0 \frac{\partial \mathcal{L}_t}{\partial \nabla \rho_0} \cdot \mathbf{N} \operatorname{div} \mathbf{F}^{-1} \quad \text{on } \Sigma_t, \\ {}^d\mathbb{T}^d \mathbf{N} = 0, \quad {}^d\mathbf{T}^d \mathbf{N} = \rho_0 \frac{\partial \mathcal{L}_t}{\partial {}^d \nabla \rho_0} \cdot {}^d \mathbf{N} \operatorname{div} {}^d \mathbf{F}^{-1} \quad \text{on } {}^d\Sigma_t \end{aligned} \quad (3.42)$$

represent the static boundary conditions of Eshelbian and Newtonian type. Using the identities $\operatorname{div}(J \mathbf{F}^{-1}) = 0$ and $\operatorname{div}({}^d J {}^d \mathbf{F}^{-1}) = 0$ ($J = \det \mathbf{F}$, ${}^d J = \det {}^d \mathbf{F}$), the boundary conditions (Eq. (3.42), second and fourth terms) can be transformed into

$$\begin{aligned} \mathbf{T} \mathbf{N} = -\rho_0 \frac{\partial \mathcal{L}_t}{\partial \nabla \rho_0} \cdot \mathbf{N} \nabla \ln J \mathbf{F}^{-1} \quad \text{on } \Sigma_t, \\ {}^d\mathbf{T}^d \mathbf{N} = -\rho_0 \frac{\partial \mathcal{L}_t}{\partial {}^d \nabla \rho_0} \cdot {}^d \mathbf{N} {}^d \nabla \ln {}^d J {}^d \mathbf{F}^{-1} \quad \text{on } {}^d\Sigma_t. \end{aligned} \quad (3.43)$$

Under the absence of relevant changes in the mass density and/or of the determinants of \mathbf{F} and ${}^d\mathbf{F}$ the conditions (3.43) lead to the homogeneous boundary conditions $\mathbf{T} \mathbf{N} = 0$ and ${}^d\mathbf{T}^d \mathbf{N} = 0$.

If, in turn, the conditions (3.42) are satisfied, then Eq. (3.41) reduces to the following inequality

$$\delta I_t = \int_{\tilde{\Sigma}_t} \int_T \left(\frac{\partial \mathcal{L}_t}{\partial \nabla d} \cdot \mathbf{N} \delta d + \frac{\partial \mathcal{L}_t}{\partial {}^d \nabla d} \cdot {}^d \mathbf{N} \delta^d d \right) \rho_0 dS dt \geq 0. \quad (3.44)$$

This inequality has a close correlation with the inequality in fracture mechanics stating that the body with cracks can only be in stable equilibrium if the variation of its total energy is not negative (Stumpf and Le,

1990). It represents the driving force due to thermodynamically unstable states caused by the evolution of defects in an inelastically deformed body. Upon increasing the temperature the material can lower its free energy by the reduction and rearrangement of defects. This process leading to energetically more favourable configurations is, in particular, connected with the annihilation of defects and dislocations.

4. Dissipation inequality

The dissipation (Clausius–Duhem) inequality results in restrictions on the constitutive equations and it determines the permissible processes for the body. Using a Helmholtz free energy formulation the Newtonian–Eshelbian version of the dissipation condition can be obtained from the sufficiency condition for the action integral (3.1) (cf. Stumpf and Saczuk, 2000). Within the method of equivalent integrals (Lovelock and Rund, 1975) we have to construct a function Λ_t (a counterpart of the total derivative) defined on

$$\dot{x}^i = x^i(\mathbf{X}, \mathbf{D}, t), \quad \theta = \theta(\mathbf{X}, \mathbf{D}, t). \quad (4.1)$$

(Here we assume that \mathcal{L}_t is dependent also on temperature θ and its gradients $\nabla\theta$ and ${}^d\nabla\theta$.) This function Λ_t , which is independent of the choice of the sub-space (4.1), is the integrand of a new action integral

$$\bar{I}_t = \int_G \int_T \bar{\mathcal{L}}_t(\mathbf{X}, \mathbf{D}) dV dt,$$

where $\bar{\mathcal{L}}_t(\mathbf{X}, \mathbf{D}) = \mathcal{L}_t(\mathbf{X}, \mathbf{D}) - \Lambda_t(\mathbf{X}, \mathbf{D})$. Then the integral \bar{I}_t , by definition, provides an extreme value for the same solutions as those of the original problem defined by $I_t = \int_G \int_T \mathcal{L}_t dV dt$.

Within the argumentation presented in Stumpf and Saczuk (2000) the sufficiency condition for the action integral (3.1) can be reduced (neglecting the heat supply) to the following inequality,

$$\begin{aligned} \rho_0(\eta\dot{\theta} + \dot{\Psi}) - (\mathbf{T} + {}^d\mathbf{T}) \cdot (\dot{\mathbf{F}} + {}^d\dot{\mathbf{F}}) - (\mathbb{T} + {}^d\mathbb{T}) \cdot (\dot{\mathbb{F}} + {}^d\dot{\mathbb{F}}) + \left(\frac{\partial \mathcal{L}_t}{\partial \nabla d} + \frac{\partial \mathcal{L}_t}{\partial {}^d \nabla d} \right) \cdot (\nabla \dot{d} + {}^d \nabla \dot{d}) \\ + \theta^{-1}(\nabla\theta + {}^d\nabla\theta) \cdot (\mathbf{H} + {}^d\mathbf{H}) \leq 0, \end{aligned} \quad (4.2)$$

where $\Psi = \mathcal{L}_t - \theta$ is the Helmholtz free energy, η the entropy, \mathbb{F} and ${}^d\mathbb{F}$ the configurational gradients, \mathbf{H} and ${}^d\mathbf{H}$ the heat flux vectors.

The inequality (4.2), similar to the one postulated by Gurtin and Podio-Guidugli (1998), has been derived from the local changes in the mass and defect densities.

5. A nonlocal constitutive model accounting for the evolution of the defect density

To complete the set of equations defining a thermodynamical theory of continuum mechanics we have to postulate appropriate constitutive equations. In the following we select as independent variables (see Green and Laws (1967) for a discussion on the choice of independent variables) the macro- and microstrain tensors \mathbf{E} and ${}^d\mathbf{E}$, the defect density d , its macrogradient ∇d and the temperature θ . According to the principle of equipresence we assume the following constitutive equations:

$$\begin{aligned}
\Psi &= \hat{\Psi}(\mathbf{E}, {}^d\mathbf{E}, d, \nabla d, \theta) \\
\mathbf{S} &= \hat{\mathbf{S}}(\mathbf{E}, {}^d\mathbf{E}, d, \nabla d, \theta) \\
{}^d\mathbf{S} &= {}^d\hat{\mathbf{S}}(\mathbf{E}, {}^d\mathbf{E}, d, \nabla d, \theta) \\
\eta &= \hat{\eta}(\mathbf{E}, {}^d\mathbf{E}, d, \nabla d, \theta) \\
\mathbf{H} &= \hat{\mathbf{H}}(\mathbf{E}, {}^d\mathbf{E}, d, \nabla d, \theta)
\end{aligned} \tag{5.1}$$

for the Helmholtz free energy, the second Piola–Kirchhoff stress tensor, the entropy and the heat flux vector.

The following simplified form of the first term of Eq. (5.1) can be assumed (see also Fried and Gurtin (1994) and Frémond and Nedjar (1996))

$$\Psi = \Psi_{e-p}(\mathbf{E}, {}^d\mathbf{E}, \theta) + \Psi_d(d, \nabla d),$$

where Ψ_{e-p} is the strain energy potential, and Ψ_d can be defined by an initial damage threshold, its displacement and viscosity effects of damage, whenever d can be identified with the damage scalar variable.

The constitutive equations (5.1) cannot be arbitrary functions of their arguments, but have to satisfy the entropy inequality for every thermodynamical process compatible with Eq. (5.1) (cf. Coleman and Noll, 1963). By differentiating Ψ with respect to time and substituting the resulting expression into the dissipation inequality (4.2), we obtain, as a result of the nonnegative requirement of the entropy production, the following constitutive equations

$$\begin{aligned}
\mathbf{S} &= \rho_0 \frac{\partial \Psi}{\partial \mathbf{E}}, \quad {}^d\mathbf{S} = \rho_0 \frac{\partial \Psi}{\partial {}^d\mathbf{E}}, \\
\frac{\partial \mathcal{L}_t}{\partial \nabla d} &= -\rho_0 \frac{\partial \Psi}{\partial \nabla d}, \quad \frac{\partial \mathcal{L}_t}{\partial {}^d\nabla d} = -\rho_0 \frac{\partial \Psi}{\partial {}^d\nabla d}, \\
\eta &= -\frac{\partial \Psi}{\partial \theta}, \quad \frac{\partial \Psi}{\partial \nabla \theta} = \frac{\partial \Psi}{\partial {}^d\nabla \theta} = 0.
\end{aligned} \tag{5.2}$$

Using Eq. (5.2) the inequality (4.2) reduces to the following objective form

$$-\mathbf{S} \cdot {}^d\dot{\mathbf{E}} - {}^d\mathbf{S} \cdot \dot{\mathbf{E}} - \mathbb{S} \cdot {}^d\dot{\mathbb{E}} - {}^d\mathbb{S} \cdot \dot{\mathbb{E}} + \frac{\partial \mathcal{L}_t}{\partial \nabla d} \cdot {}^d\nabla \dot{d} + \frac{\partial \mathcal{L}_t}{\partial {}^d\nabla d} \cdot \nabla \dot{d} + \theta^{-1} (\nabla \theta + {}^d\nabla \theta) \cdot (\mathbf{H} + {}^d\mathbf{H}) \leq 0 \tag{5.3}$$

taking into account mechanical and thermal contributions to the entropy production. In reducing the term $(\mathbb{T} + {}^d\mathbb{T}) \cdot (\dot{\mathbb{F}} + {}^d\dot{\mathbb{F}})$ in Eq. (4.2) to $\mathbb{S} \cdot {}^d\dot{\mathbb{E}} + {}^d\mathbb{S} \cdot \dot{\mathbb{E}}$ in Eq. (5.3), we used the following definitions (cf. Eq. (3.12)):

$$\mathbb{S} = \rho_0 \Psi \mathbf{1} - \mathbf{E} \frac{\partial \Psi}{\partial \mathbf{E}}, \quad {}^d\mathbb{S} = \rho_0 \Psi^d \mathbf{1} - {}^d\mathbf{E} \frac{\partial \Psi}{\partial {}^d\mathbf{E}}.$$

For simplicity, we neglect the temperature influence and assume that $\Psi = \Psi(\mathbf{E}, {}^d\mathbf{E}, d, \nabla d)$ has the derivatives (first and second terms of Eq. (5.2)), while the thermodynamic conjugate force S_d corresponding to d and ∇d is defined as the nonlocal gradient-type constitutive equation

$$S_d = \rho_0 \frac{\partial \Psi}{\partial d} = \rho_0 \left[\frac{\partial \Psi}{\partial d} - \frac{1}{\rho_0} \operatorname{div} \left(\rho_0 \frac{\partial \Psi}{\partial \nabla d} \right) \right].$$

Time derivatives of \mathbf{S} , ${}^d\mathbf{S}$ and S_d lead to

$$\dot{\mathbf{S}} = \mathbb{C} \cdot \dot{\mathbf{E}} + {}^x \mathbb{C} \cdot {}^d\dot{\mathbf{E}} + \mathbb{C}_d \dot{d}, \tag{5.4}$$

$${}^d\dot{\mathbf{S}} = {}^d_x \mathbb{C} \cdot \dot{\mathbf{E}} + {}^d \mathbb{C} \cdot {}^d\dot{\mathbf{E}} + {}^d \mathbb{C}_d \dot{d}, \tag{5.5}$$

$$\dot{S}_d = \mathbb{C}_d^T \cdot \dot{\mathbf{E}} + {}^d\mathbb{C}_d^T \cdot {}^d\dot{\mathbf{E}} + C_d \dot{d}, \quad (5.6)$$

where

$$\mathbb{C} = \frac{\partial \mathbf{S}}{\partial \mathbf{E}}, \quad {}^x\mathbb{C} = \frac{\partial \mathbf{S}}{\partial {}^d\mathbf{E}}, \quad {}^d\mathbb{C} = \frac{\partial {}^d\mathbf{S}}{\partial \mathbf{E}}, \quad {}^d\mathbb{C} = \frac{\partial {}^d\mathbf{S}}{\partial {}^d\mathbf{E}},$$

$$\mathbb{C}_d = \frac{\partial \mathbf{S}}{\partial d} = \frac{\partial S_d}{\partial \mathbf{E}} = \mathbb{C}_d^T, \quad {}^d\mathbb{C}_d = \frac{\partial {}^d\mathbf{S}}{\partial d} = \frac{\partial S_d}{\partial {}^d\mathbf{E}} = {}^d\mathbb{C}_d^T, \quad C_d = \frac{\partial^2 \Psi}{\partial d^2}.$$

Let us assume an evolution law for ${}^d\dot{\mathbf{E}}$ and d in the form

$${}^d\dot{\mathbf{E}} = \dot{\lambda} \frac{\partial \Phi}{\partial {}^d\mathbf{S}}, \quad \dot{d} = \dot{\lambda} \frac{\partial \Phi}{\partial S_d}, \quad (5.7)$$

which close the system of equations, and where $\Phi = \Phi({}^d\mathbf{E}, {}^d\mathbf{S}, d, \nabla d, S_d)$ is an evolution (dissipation) potential. The above evolution equations represent a class of purely resistive materials. With the time derivative of Φ ,

$$\dot{\Phi} = \frac{\partial \Phi}{\partial {}^d\mathbf{E}} \cdot {}^d\dot{\mathbf{E}} + \frac{\partial \Phi}{\partial {}^d\mathbf{S}} \cdot {}^d\dot{\mathbf{S}} + \frac{\partial \Phi}{\partial d} \dot{d} + \frac{\partial \Phi}{\partial S_d} \dot{S}_d,$$

with the Eqs. (5.5)–(5.7) and with the condition $\dot{\Phi} = 0$ one can determine the consistency parameter $\dot{\lambda}$,

$$\dot{\lambda} = -D^{-1} \left(\frac{\partial \Phi}{\partial {}^d\mathbf{S}} \cdot {}^d\mathbb{C} + \frac{\partial \Phi}{\partial S_d} \mathbb{C}_d^T \right) \cdot \dot{\mathbf{E}}, \quad (5.8)$$

where the dominator D is given by

$$D = \frac{\partial \Phi}{\partial {}^d\mathbf{E}} \cdot \frac{\partial \Phi}{\partial {}^d\mathbf{S}} + \frac{\partial \Phi}{\partial d} \frac{\partial \Phi}{\partial S_d} + \frac{\partial \Phi}{\partial {}^d\mathbf{S}} \cdot \left({}^d\mathbb{C} \cdot \frac{\partial \Phi}{\partial {}^d\mathbf{S}} + {}^d\mathbb{C}_d \frac{\partial \Phi}{\partial S_d} \right) + \frac{\partial \Phi}{\partial S_d} \left({}^d\mathbb{C}_d^T \cdot \frac{\partial \Phi}{\partial {}^d\mathbf{S}} + C_d \frac{\partial \Phi}{\partial S_d} \right).$$

Finally, we obtain the rate constitutive equation for the macro second Piola–Kirchhoff stress tensor,

$$\dot{\mathbf{S}} = \left[\mathbb{C} - D^{-1} \left({}^x\mathbb{C} \cdot \frac{\partial \Phi}{\partial {}^d\mathbf{S}} + \frac{\partial \Phi}{\partial S_d} \mathbb{C}_d \right) \otimes \left(\frac{\partial \Phi}{\partial {}^d\mathbf{S}} \cdot {}^d\mathbb{C} + \mathbb{C}_d^T \frac{\partial \Phi}{\partial S_d} \right) \right] \cdot \dot{\mathbf{E}}. \quad (5.9)$$

If $\mathbf{A} = {}^x\mathbb{C} \cdot \frac{\partial \Phi}{\partial {}^d\mathbf{S}} + \frac{\partial \Phi}{\partial S_d} \mathbb{C}_d$ can be approximated by $\mathbf{A} = \text{tr} \mathbf{A} \mathbf{1}$ then Eq. (5.9) can be rewritten as

$$\dot{\mathbf{S}} = \left[1 - D^{-1} \left({}^x\mathbb{C} \cdot \frac{\partial \Phi}{\partial {}^d\mathbf{S}} + \frac{\partial \Phi}{\partial S_d} \mathbb{C}_d \right) \cdot \mathbb{C}^{-1} \cdot \left(\frac{\partial \Phi}{\partial {}^d\mathbf{S}} \cdot {}^d\mathbb{C} + \mathbb{C}_d^T \frac{\partial \Phi}{\partial S_d} \right) \right] \mathbb{C} \cdot \dot{\mathbf{E}} = (1 - k) \mathbb{C} \cdot \dot{\mathbf{E}}, \quad (5.10)$$

where

$$k = D^{-1} \left({}^x\mathbb{C} \cdot \frac{\partial \Phi}{\partial {}^d\mathbf{S}} + \frac{\partial \Phi}{\partial S_d} \mathbb{C}_d \right) \cdot \mathbb{C}^{-1} \cdot \left(\frac{\partial \Phi}{\partial {}^d\mathbf{S}} \cdot {}^d\mathbb{C} + \mathbb{C}_d^T \frac{\partial \Phi}{\partial S_d} \right)$$

is a scalar-valued variable.

If we neglect in Eq. (5.9) the inelastic microcontribution induced by ${}^d\mathbf{E}$, and if we take into account that $\mathbb{C}_d = \mathbb{C} \cdot \frac{\partial \mathbf{E}}{\partial d}$ then

$$\dot{\mathbf{S}} = \left(1 - \frac{\frac{\partial \Phi}{\partial S_d} \frac{\partial \mathbf{E}}{\partial d} \cdot \mathbb{C} \cdot \frac{\partial \mathbf{E}}{\partial d}}{C_d \frac{\partial \Phi}{\partial S_d} + \frac{\partial \Phi}{\partial d}} \right) \mathbb{C} \cdot \dot{\mathbf{E}} \quad (5.11)$$

is the desired result showing a definite influence of the defect density on the rate-dependent constitutive relation.

6. Conclusion

In this paper we proposed a unified description of inelastic material behaviour accounting for the evolution of defect and mass densities based on the concept of a generalized oriented continuum.

Applying variational arguments, balance laws, boundary and transversality conditions of inelastic materials were derived within an irreversible thermodynamic theory with special emphasis on the changes induced by mass and defect densities. Various special cases of the presented formulation are discussed and a number of correlations with the results in hydrodynamics and phase transitions are considered.

The Helmholtz free energy functional, the dissipation potential and the evolution equations for microstrain tensor and defect density are used to derive rate-dependent constitutive equations and a nonlocal constitutive damage model of Kachanov's type.

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