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ON NONLOCAL GRADIENT MODEL OF INELASTIC HETEROGENEOUS MEDIA

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The aim of this paper is to investigate the influence of nonlocality on the physical and material field equations of heterogeneous media. Taking into account that plastic deformations in metals or damage in brittle and ductile materials are governed by physical mechanisms observed on levels with different lengthscales, we introduce a 6-dimensional kinematical concept with two locally defined vectors to model the material behaviour on a macro- and meso- or microlevel.
Using a variational procedure the physical and material balance laws, boundary and transversality conditions are derived for macro- and microdeformations of heterogeneous media. The dissipation inequality including relaxation terms for transport processes is presented. The constitutive equations are formulated with macro- and microstrain measures, their gradients and time rates, and the anisotropy tensor as arguments, where the latter can be considered as a coupling measure between the deformed macrostates with compatible microstates.
The model presented in this paper delivers a framework, which enables one to derive various nonlocal and gradient theories by introducing simplifying assumptions. As the special case a solid-void model is considered.

Key words: microstructure, nonlocal inelasticity, gradient theory, configurational forces

Dedicated to Professor Czesław Woźniak on the occasion of his 70^{th} birthday

1. Introduction

In the lifetime oriented design and analysis of engineering structures increasing research efforts were made during the last couple of years to overcome essential deficiencies of local models of continuum mechanics, especially in the fields of finite elastoplasticity, damage and fracture mechanics (cf. Nowacki, 1986). These deficiences can be observed in finite element solutions based on local models, which exhibit a strong mesh-dependency whenever a strain localization occurs, or even they are not able to simulate problems with scale effects (cf. Bažant and Ožbolt, 1990). The reason for this is the fact that the plastic deformations or damage of material bodies are governed by physical mechanisms on levels with different lengthscales, on a macro- and meso- or microlevel, and the interaction of these phenomena can be described appropriately only by nonlocal theories.

The inescapable influence of the nonlocality to classical notions as stress at a point depending on the state of the whole body was already noted by Duhem in 1893. Since then, many nonlocal models of continuum mechanics were proposed (cf. Rogula, 1973), which can be grouped according to their essential feature. Here, we can mention only a few papers. Taking into account that the plastic deformation process is governed by dislocation motion Bilby et al. (1955), Kröner (1960), Kunin (1968), Krumhansl (1968), Valanis (1969), Le and Stumpf (1996a,b) used as kinematical concept a non-Euclidean space structure to model the influence of dislocation motion on the macrodeformation of elastic-plastic bodies. In an alternative approach a material particle can be equipped with additional degrees of freedom as the director theories of Ericksen (1961), Toupin (1964) and Mindlin (1964), the multipolar theory of Green and Rivlin (1964a) and the micropolar theory of Eringen (1964) (cf. Woźniak, 1973). The third category of nonlocal models is characterized by including higher-order gradients of displacement and velocity as in the models of Toupin (1962), Mindlin and Tiersten (1962), and Green and Rivlin (1964b). In the above mentioned papers additional balance laws were introduced. In the next category the nonlocal interactions were resolved by introducing certain integral terms into the balance laws without postulating additional laws. Here, we have to mention the theories of Edelen (1969), Eringen and Edelen (1972). A theory with explicit dependence on nonlocality, but with additional laws for nonlocal ingredients was given by Gurtin and Williams (1971a).

Recent results have shown that the locality assumption leads to significant errors in the treatment of the energetic description of dislocations within cohesive zone models (Miller et al., 1998). The cohesive zone models, which constitute a bridge between the microscopic and macroscopic modelling of material behavior, were first proposed by Peierls (1940) to describe dislocations and by Barenblatt (1962) to model fracture processes.

Continuum theories, including long-range interactions, have been investigated by Kunin (1982, 1983), Gurtin and Williams (1971b), and Edelen (1976). There are different approaches to the problem of describing nonlocal interactions, but common is to postulate balance equations for the whole body and not for an arbitrary part. Corresponding local equations are only valid after the incorporation of nonlocal residulas accounting for the long-range interactions.

The need for nonlocal models (Maugin, 1979; Eringen, 1992) in damage mechanics and finite elastoplasticity became evident, when during the last decade numerical simulations of experimental data were not able to predict appropriately size effects, and the numerical results obtained by FE methods based on local models exhibited a strong mesh-dependency (e.g. Bažant, 1991; Roehl and Ramm, 1996; Miehe, 1998; Schieck et al., 1999). To overcome these deficiences an integral enhancement of the strain measures (Bažant and Pijaudier, 1988) and a gradient enhancement of the strain or hardening parameters (e.g. de Borst and Mülhaus, 1992; de Borst et al., 1996; Fleck and Hutchinson, 1997; Gao et al., 1999) were introduced into the local models to overcome the obvious deficiencies of numerical procedures. Consistent nonlocal theories of the gradient type in finite elastoplasticity were proposed by Naghdi and Srinivasa (1993) and Le and Stumpf (1996a,b), where the dislocation density tensor as an additional microvariable has to satisfy own balance law of microforces.

It is well-known that in the presence of fields of dislocations, voids, microcracks and other defects there exist only locally defined vector fields and that an appropriate corresponding kinematical model is a manifold with torsion and curvature. Also the classical Euclidean gradient operator has to be replaced by the so-called connection. In an interesting paper Rakotomamana (2001) has shown that the results obtained by ultrasonic in site measurements of the state of damage in engineering structures cannot be interpreted correctly, if the underlying theory is based on a gradient theory with the classical operator and not using a non-Euclidean manifold.

In order to model continua with defects on two levels with different length-scales, the macro- and mesolevel, Stumpf and Saczuk (2000, 2001) introduced a 6-dimensional model with two locally defined vectors, where one vector represents the macroposition and the other a local vector on the microlevel with a physical interpretation according to the underlying problem. A variational approach enables then derivation of the balance laws for macro- and microforces with two different non-Euclidean differential operators.

The aim of this paper is to present a thermodynamical framework for the modelling of two-scale inelastic processes in heterogeneous media.

The structure of the paper is as follows. In Section 2 we discuss first some physical interpretations of the locally defined microvector. Then, we shortly recall the basic kinematical results outlined in detail in Stumpf and Saczuk (2000, 2001). Also we define the deformation induced anisotropy tensors representing the microstructural changes in the material anisotropy. In Section 3 we present a variational-based derivation of the physical and material balance laws on the macro- and microlevel, where also the gradients of the deformation measures on both levels are taken into account leading to the second-order first Piola-Kirchhoff and Eshelby stress tensor in the balance laws, boundary and transversality conditions. Also, in Section 3, we include viscous contributions of the deformation measure and its gradient and derive their contribution to the balance laws. In Section 4 the dissipation inequality is considered, and in Section 5 we discuss the constitutive modelling taking into account the strain measures on both levels and their gradients and rates, the anisotropy tensor, temperature and its gradient as well as its rate. In Section 6 we discuss the special case of a solid-void continuum model and finally, in Section 7, we present the conclusion of the paper.

2. Kinematics of a heterogeneous body

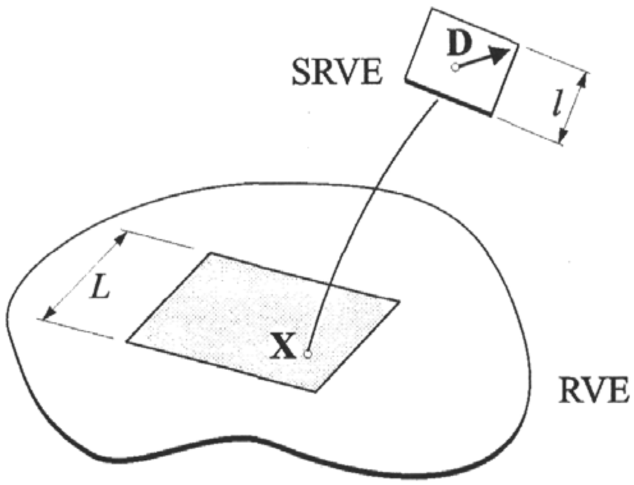

Fig. 1.

Let us assume that in the reference configuration at the time $t = 0$ the material body, which models appropriately inelastic phenomena in solids, occupies a regular region B_0 in the three-dimensional space. For the choice of an appropriate kinematical model let us consider in the body B at the time instant t a representative volume element (RVE) on the macroscale and a representative sub-volume element (SRVE) with distributed microdefects on a mesoscale (Fig. 1). Correspondingly, we shall model the body B_t by a generalized 3-dimensional oriented continuum $\mathfrak{B}$ endowed at each point with an internal structure. Following the picture of a two-level description with RVE and SRVE, we introduce in the reference configuration C_0 a pair of two locally defined vectors $(\boldsymbol{X}, \boldsymbol{D})$, where the macrovector $\boldsymbol{X}$ can be identified with the location of the material particle in the macrocontinuum (RVE) and the microvector $\boldsymbol{D}$ with the location in the microcontinuum (SRVE) or orientation of the crystalographic structure depending on the problem under consideration.

2.1. Background information in a (sub-)microscopic description of the variable D

We provide here some additional information which justifies the choice of the variable $\boldsymbol{D}$ at different spatial scales and give its physical interpretation. We observe that for inelastic behaviour of materials, a number of microstructural features of their motion can always be seen with increasing details at finer scales of observation. While the body appears quite smooth on the macroscale, its permanent deformation at finer scales turns out to be discontinuous. With reference to the microscopic description of the body, in the vicinity of an arbitrary point $\boldsymbol{X}$ of $\mathfrak{B}$ we consider a propagating dislocation segment with the tangent vector $\boldsymbol{\xi}$, velocity $\boldsymbol{\nu}$ and Burgers's vector $\boldsymbol{b}$ during some time interval. The discrete motion of dislocations within the vicinity of $\boldsymbol{X}$ can be modelled, within an idealized mechanistic model in the RVE, by the dislocation kinetics that depends on the dislocation density d. In this model the dislocation functional d, assumed to be a continuous function of $\boldsymbol{X}$, $\boldsymbol{\xi}$, $\boldsymbol{\nu}$, $\boldsymbol{b}$ and t, describes the probable number of dislocations in the sub-volume element $\mathfrak{B}_R$ attached to the point $\boldsymbol{X}$.

The vector $\boldsymbol{D}(\boldsymbol{X}, t)$, the displacement between atoms in $\mathfrak{B}_R$ with respect to $\boldsymbol{X}$, can be defined by (Stout, 1981)

$$\boldsymbol{D}(\boldsymbol{X}, t) = \int_{\mathfrak{B}_R} \boldsymbol{b}\boldsymbol{\xi} \times \Big\{ \boldsymbol{\nu} d + \boldsymbol{b}^\star [\partial_t d + \nabla^\star \cdot (\overline{\boldsymbol{\nu}} d)] \Big\} \, dV_R \tag{2.1}$$

where the first term of the integrand describes the contribution from the dislocation motion, and the second term, from the changes of the dislocation density. Moreover, in Eq. (2.1) we denote by dV_R the sub-volume element equal to $d\boldsymbol{b} d\boldsymbol{\xi} d\boldsymbol{\nu} d\boldsymbol{\chi} dt$ with $\boldsymbol{\chi}$ denoting the position of the atoms at the time t, by $\boldsymbol{b}^\star$ the lumped vector modelling the displacements of the neighbouring atoms when the changes of the dislocation density take place, and by $\overline{\boldsymbol{\nu}}$ the velocity of the transported dislocation configuration changes in B_R. Also, the notation $\nabla^\star$ stands for the spatial differential operator with respect to $\boldsymbol{X}$ and ∂_t for the time part.

In the context of the theory of structured solids developed by Naghdi and Srinivasa (1993, 1994) one can represent the periodic arrangement of the crystal lattice of crystals at each particle $\boldsymbol{X}^\star$ of $\mathfrak{B}^\star \subset \mathfrak{B}$ by means of the lattice vectors $\boldsymbol{D}^\star$, non-complanar by definition in any time interval. Then the vector $\boldsymbol{D}(\boldsymbol{X}, t)$, called by them the lattice director, can be expressed as a spatial average of the local values of the lattice vector by

$$\boldsymbol{D}(\boldsymbol{X}, t) = \frac{1}{V^\star} \int_{\mathfrak{B}^\star} \boldsymbol{D}^\star \, dV \tag{2.2}$$

where $V^\star$ is the volume of any arbitrary material volume $\mathfrak{B}^\star$ of $\mathfrak{B}$ in the reference configuration. In Eq. (2.2) $\boldsymbol{D}^\star$ is evaluated at the point $\boldsymbol{X}$ in the local sub-representative volume element (SRVE).

The volume average $\overline{\boldsymbol{D}}$ of the microvector field $\boldsymbol{D}$ defined in the RVE with cracks is defined as

$$\overline{\boldsymbol{D}}(t) = \frac{1}{V} \lim_{\delta \to 0} \int_{V_\delta} \boldsymbol{D}(\boldsymbol{X}, t) \, dV \tag{2.3}$$

where V is the volume of the RVE without the cracks, $V_\delta = V - \sum_i V_{ci}$ and the volume V_{ci} is the volume of the ith region with cracks represented by surfaces of discontinuity (Costanzo et al., 1996).

In the light of these remarks, the vector $\boldsymbol{D}$, in special cases, can be understand as the atomic displacement, (2.1), or the lattice director, (2.2). On the other hand, within the generalized model of the oriented continuum (Stumpf and Saczuk, 2000), the correlation between properties of a statistical mechanics and those of the field theory (Girifalco, 1973; Wilson and Kogut, 1974) leads to another physical interpretation of the vector $\boldsymbol{D}$.

The system we imagine now is a SRVE, attached at the point $\boldsymbol{X}$ of the RVE, of distributed N discrete dislocations with Burgers's vectors $\boldsymbol{b}_j$. The behaviour of the system, usually defined by means of a Hamiltonian, is determined mainly by the type of interactions present in the Hamiltonian and the strengths of the corresponding coupling constants. In this case, each dislocation configuration has a particular energy described, by assumption, by a Hamiltonian

$$H = a \sum_j \sum_k \boldsymbol{b}_j \cdot \boldsymbol{b}_k$$

accounting only for the nearest-neighbour dislocation coupling, where a is the dislocation-dislocation interaction parameter. Macroscopic degrees of freedom are the values of the dislocation functional $W(\boldsymbol{X},\cdot)$ (Stumpf and Saczuk, 2000) at macroscopically separated points.

If the SRVE is immersed in the external force field $\boldsymbol{B}$ then the Hamiltonian requires the additional term

$$H = a\sum_j\sum_k \boldsymbol{b}_j\cdot\boldsymbol{b}_k + \boldsymbol{B}\cdot\sum_j \boldsymbol{b}_j$$

The statistical property of the SRVE follows from the hypothesis that the probability P for a particular dislocation vector configuration is defined by

$$P = \exp(-\beta H)$$

where $\beta = (k_B\theta)^{-1}$, θ is the temperature and k_B the Boltzmann constant. According to the statistical physics methodology, the thermodynamics of the SRVE is deduced from the partition function

$$Z = \sum_{\{config\}} \exp(-\beta H)$$

where the sum runs over all possible dislocation configurations of the SRVE.

Using the free energy concept

$$\Psi = -k_B\theta\ln Z$$

an average defect or distortion vector (of the lattice, if distinguished, of the SRVE) per site can be expressed as

$$\overline{\boldsymbol{b}} = \frac{1}{N}\frac{\partial\Psi}{\partial\boldsymbol{B}} = \Big\langle N^{-1}\sum_j \boldsymbol{b}_j\Big\rangle$$

where $\langle\ldots\rangle$ stands for the sum over configurations.

To define an analytical model of the RVE we shall identify $\overline{\boldsymbol{b}}$ with the director vector $\boldsymbol{D}$ if $|\overline{\boldsymbol{b}}| \neq 0$. Using this macro-micro vector concept as the point of issue, we have to introduce a kinematical structure of $\mathfrak{B}$ general enough to describe inelastic material behaviour with dislocation motion and evolving macro- and microdefects. This goal can be reached by choosing a non-Euclidean space structure for the body $\mathfrak{B}$.

2.2. A nonlocal geometric setting for the body

To make the paper self-contained, we recall some basic results of the kinematical model introduced in Stumpf and Saczuk (2000) and Saczuk et al. (2001).

We assume that the deformation χ_t of the body $\mathfrak{B}$ can be expressed in terms of the locally defined vectors $(\boldsymbol{X}, \boldsymbol{D})$ on the macro- and microlevel relating particles in the actual configuration C_t by means of a smooth invertible map

$$\begin{aligned} \boldsymbol{x} &= \chi_t(\boldsymbol{X}, \boldsymbol{D}) \qquad \chi_t : \mathfrak{B} \to \mathbb{E}^3 \times \mathbb{E}^3 \\ &= {}^x\chi_t(\boldsymbol{X}, \boldsymbol{D}) + {}^d\chi_t(\boldsymbol{X}, \boldsymbol{D}) \end{aligned} \tag{2.4}$$

with associated particles in the reference configuration C_0. In Eq. (2.4) ${}^x\chi_t$ may be interpreted as the macroplacement of the material particle in the RVE and ${}^d\chi_t$ as the microplacement and/or orientation of the material particle in the sub-RVE at the actual configuration C_t.

Deformation gradient

Consider the geometry of the body $\mathfrak{B}$ induced by the metric tensor $\mathcal{G}$

$$\mathcal{G}(\boldsymbol{X}, \boldsymbol{D}) = {}^xG_{JK}\boldsymbol{G}^J \otimes \boldsymbol{G}^K + {}^dG_{\Lambda\Sigma}{}^d\mathcal{G}^\Lambda \otimes {}^d\mathcal{G}^\Sigma \tag{2.5}$$

where the metric space components ${}^xG_{JK} = {}^dG_{JK}$ are state-dependent functions. Eq. (2.5) is written in a globally defined fields of adapted coframes

$$\boldsymbol{G}^K \qquad {}^d\mathcal{G}^\Sigma = {}^d\boldsymbol{G}^\Sigma + {}_rN_L^\Sigma\,\boldsymbol{G}^L \qquad {}_rN_L^\Sigma \equiv (\boldsymbol{N}_r)_L^\Sigma \tag{2.6}$$

dual to the adapted frames

$$\mathcal{G}_K = \boldsymbol{G}_K - {}_rN_K^\Lambda\,{}^d\boldsymbol{G}_\Lambda \qquad {}^d\boldsymbol{G}_\Lambda \qquad {}_rN_K^\Lambda \equiv (\boldsymbol{N}_r)_K^\Lambda \tag{2.7}$$

where

$$\boldsymbol{G}_K = \frac{\partial}{\partial X^K} \qquad {}^d\boldsymbol{G}_\Lambda = \frac{\partial}{\partial D^\Lambda} \qquad (K, \Lambda = 1, 2, 3)$$

are the natural base vectors, and

$$\boldsymbol{G}^K = dX^K \qquad {}^d\boldsymbol{G}^\Sigma = dD^\Sigma \qquad (K, \Lambda = 1, 2, 3)$$

and natural covectors. The coefficients ${}_rN_K^\Sigma$ constitute a representation of the non-linear connection $\boldsymbol{N}_r$ of the body $\mathfrak{B}$.

To define covariant differential operators on $\mathfrak{B}$, we introduce a linear connection $\nabla = [{}^x\nabla\,{}^d\nabla]$ with the macro-covariant derivative ${}^x\nabla$ and the micro-covariant derivative ${}^d\nabla$. In terms of the covariant derivatives

$$ {}^x\nabla_{\mathcal{G}_I}\mathcal{G}_J = \Gamma^K_{IJ}\mathcal{G}_K \tag{2.8} $$

and

$$ {}^d\nabla_{{}^d\boldsymbol{G}_\Sigma}{}^d\boldsymbol{G}_\Omega = \Gamma^\Lambda_{\Sigma\Omega}{}^d\boldsymbol{G}_\Lambda \tag{2.9} $$

where the coefficients Γ^K_{IJ} are the macroconnection coefficients for the sub-bundle ${}^x(T\mathfrak{B})$ and $\Gamma^\Lambda_{\Sigma\Omega}$ the microconnection coefficients for the sub-bundle ${}^d(T\mathfrak{B})$, the deformation gradient $\widetilde{\mathsf{F}}: T\mathfrak{B}_0 \to T\mathfrak{B}_t$, associated with deformation function (2.4), is defined by

$$ \widetilde{\mathsf{F}} = \nabla\boldsymbol{\chi}_t = \begin{bmatrix} {}^x\widetilde{\mathsf{F}} & {}^x_d\widetilde{\mathsf{F}} \\ {}^d_x\widetilde{\mathsf{F}} & {}^d\widetilde{\mathsf{F}} \end{bmatrix} \tag{2.10} $$

where the block components of $\widetilde{\mathsf{F}}$ are given as

$$ \begin{aligned} {}^x\widetilde{\mathsf{F}} &= {}^x\nabla\,{}^x\boldsymbol{\chi}_t = {}^x\nabla_{\mathcal{G}_K}{}^x\boldsymbol{\chi}_t \otimes \boldsymbol{G}^K \\ {}^x_d\widetilde{\mathsf{F}} &= {}^x\nabla\,{}^d\boldsymbol{\chi}_t = {}^x\nabla_{\mathcal{G}_K}{}^d\boldsymbol{\chi}_t \otimes \boldsymbol{G}^K \\ {}^d_x\widetilde{\mathsf{F}} &= {}^d\nabla\,{}^x\boldsymbol{\chi}_t = {}^d\nabla_{{}^d\boldsymbol{G}_\Lambda}{}^x\boldsymbol{\chi}_t \otimes {}^d\mathcal{G}^\Lambda \\ {}^d\widetilde{\mathsf{F}} &= {}^d\nabla\,{}^d\boldsymbol{\chi}_t = {}^d\nabla_{{}^d\boldsymbol{G}_\Lambda}{}^d\boldsymbol{\chi}_t \otimes {}^d\mathcal{G}^\Lambda \end{aligned} \tag{2.11} $$

with the Christoffel symbol objects on the macrospace ${}^x\boldsymbol{\Gamma} := (\Gamma^K_{IJ})$ and microspace ${}^d\boldsymbol{\Gamma} := (\Gamma^\Lambda_{\Sigma\Omega})$. We assume here that $\det\widetilde{\mathsf{F}} \neq 0$.

In general, the deformation gradient $\widetilde{\mathsf{F}}$ includes the relevant, taken from the mesoscale, information of the processes taking place at the microscale and defined in the adapted basis. Only on certain simplifying assumptions the above deformation measures can be reduced to the classical counterparts. There is also an additional possibility to reduce $\widetilde{\mathsf{F}}$ to the diagonal form F expressing explicitly both the macro- and microbehaviour.

Let us introduce a deformation-induced anisotropy tensor A_F and the deviation tensor B_F to transform the deformation tensor $\widetilde{\mathsf{F}}: T\mathfrak{B}_0 \to T\mathfrak{B}_t$ with block components (2.10) into the diagonal form $\mathsf{F}: {}^x(T\mathfrak{B}_0) \oplus {}^d(T\mathfrak{B}_0) \to {}^x(T\mathfrak{B}_t) \oplus {}^d(T\mathfrak{B}_t)$

$$ \mathsf{F} = \mathsf{A}_F\widetilde{\mathsf{F}}\mathsf{B}_F = \begin{bmatrix} {}^x\mathsf{F} & \mathbf{0} \\ \mathbf{0} & {}^d\mathsf{F} \end{bmatrix} \tag{2.12} $$

The deformation-induced anisotropy tensors A_F and B_F, diagonal components ${}^x\mathsf{F}$ and ${}^d\mathsf{F}$, respectively, are defined by

$$\mathbf{A}_F = \begin{bmatrix} \mathbf{I} & -{}^{x}_{d}\widetilde{\mathbf{F}}\,({}^{d}\widetilde{\mathbf{F}})^{-1} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \qquad \mathbf{B}_F = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ -({}^{d}\widetilde{\mathbf{F}})^{-1}\,{}^{d}_{x}\widetilde{\mathbf{F}} & \mathbf{I} \end{bmatrix} \tag{2.13}$$

and

$${}^{x}\mathbf{F} = {}^{x}\widetilde{\mathbf{F}} - {}^{x}_{d}\widetilde{\mathbf{F}}\,({}^{d}\widetilde{\mathbf{F}})^{-1}\,{}^{d}_{x}\widetilde{\mathbf{F}} \qquad {}^{d}\mathbf{F} = {}^{d}\widetilde{\mathbf{F}} \tag{2.14}$$

The above results demonstrate how the evolution of the microstructural changes and of the deformation process itself induce changes in the material anisotropy adjusting its internal structure to the environmentally applied loads. Therefore, the anisotropy tensor $\mathbf{A}_F$ can be considered as the coupling measure between the deformed macrostate with compatible microstates.

3. Variational-based formulation in the physical and material space

Classical continuum mechanics is based on the principle of a local action and on the assumption that the balance equations are valid for every part of a given body. The principle of the local action is not valid in nonlocal theories, when for example the stress at a material point is affected by the behaviour of other material points.

The first law of thermodynamics, balance of energy, written in incremental form for changes of an arbitrary system $\mathfrak{B}_R$ of $\mathfrak{B}$ in a time interval Δt is assumed in the form

$$\Delta U = \Delta Q + \Delta W \tag{3.1}$$

where ΔU is the change of the internal energy of $\mathfrak{B}_R$, ΔQ the internal-external heat transported to $\mathfrak{B}_R$, and ΔW the external (mechanical) work done on $\mathfrak{B}_R$ in the time Δt.

The physical terms in (3.1) will be defined in the subsequent subsections, and the second law of thermodynamics for the corresponding entropy flux in Section 4.

Variational formulation

We assume the following form for the second order functional

$$I_t = \int\limits_G \mathcal{L}(\boldsymbol{\alpha}, \boldsymbol{\beta})\rho_0 \, dV \tag{3.2}$$

where $\boldsymbol{\alpha} = \{\boldsymbol{X}, \boldsymbol{D}, \boldsymbol{x}\}$ and $\boldsymbol{\beta} = \{\mathsf{F}, \nabla\mathsf{F}\}$. The argument $\boldsymbol{D}$ represents the director vector and ρ_0 the reference mass density. The integral functional $\mathcal{L}(\boldsymbol{\alpha}, \boldsymbol{\beta})$ in (3.2), called the Lagrangian (deformation energy) density, is assumed as a smooth map

$$\mathcal{L}: \ \mathbb{E}^6 \times J^2(\mathbb{E}^6) \to \mathbb{R}$$

with $J^2(\cdot)$ being the second jet bundle, and G denotes a fixed, closed and simply-connected region in the 6-dimensional space of $(\boldsymbol{X}, \boldsymbol{D})$, 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 (3.2) is defined by

$$dV = \sqrt{\Gamma}\ d\boldsymbol{X} d\boldsymbol{D} = \sqrt{\Gamma}\ dX^1 dX^2 dX^3 dD^1 dD^2 dD^3 \tag{3.3}$$

where Γ is the determinant of the metric tensor $\boldsymbol{\mathcal{G}}$ according to (2.5).

The variational problem consists of finding the stationary values of the functional I_t in some class of the functions $\boldsymbol{x} = \boldsymbol{\chi}_t(\boldsymbol{X}, \boldsymbol{D})$ defined over G. The smoothness required for the stationary values of (3.2) is strictly correlated with the problem under consideration.

To obtain the explicite variational identity for $\mathcal{L}$ we introduce the first Piola-Kirchhoff macro-micro stress tensor defined by

$$\mathsf{T} = -\frac{\partial \mathcal{L}}{\partial \mathsf{F}} \qquad \text{or} \qquad ({}^{x}\mathsf{T}, {}^{d}\mathsf{T}) = \Big(-\frac{\partial \mathcal{L}}{\partial^{x}\mathsf{F}}, -\frac{\partial \mathcal{L}}{\partial^{d}\mathsf{F}}\Big) \tag{3.4}$$

the macro-micro couple-stress tensor

$$\mathsf{M} = -\frac{\partial \mathcal{L}}{\partial \nabla\mathsf{F}} \qquad \text{or} \qquad ({}^{x}\mathsf{M}, {}^{d}\mathsf{M}) = \Big(-\frac{\partial \mathcal{L}}{\partial^{x}\nabla^{x}\mathsf{F}}, -\frac{\partial \mathcal{L}}{\partial^{d}\nabla^{d}\mathsf{F}}\Big) \tag{3.5}$$

the Eshelbian macro-micro stress tensor

$$\mathbb{T} = -\mathcal{L}\mathsf{I} - \mathsf{T}^{\top}\mathsf{F} \tag{3.6}$$

or

$$({}^{x}\mathbb{T}, {}^{d}\mathbb{T}) = (-\mathcal{L}\,{}^{x}\mathsf{I} - {}^{x}\mathsf{T}^{\top}\,{}^{x}\mathsf{F},\ -\mathcal{L}\,{}^{d}\mathsf{I} - {}^{d}\mathsf{T}^{\top}{}^{d}\mathsf{F})$$

the external body macro-micro force vector

$$\boldsymbol{f} = \frac{\partial \mathcal{L}}{\partial \boldsymbol{x}} \qquad \text{or} \qquad ({}^{x}\boldsymbol{f}, {}^{d}\boldsymbol{f}) = \Big(\frac{\partial \mathcal{L}}{\partial^{x}\boldsymbol{\chi}_t}, \frac{\partial \mathcal{L}}{\partial^{d}\boldsymbol{\chi}_t}\Big) \tag{3.7}$$

and the macroinhomogeneity macro-micro force vector by

$$\mathsf{f} = \nabla\mathcal{L} \qquad \text{or} \qquad ({}^x\mathsf{f},\, {}^d\mathsf{f}) = ({}^x\nabla\mathcal{L},\, {}^d\nabla\mathcal{L}) \tag{3.8}$$

The integral version of the second order functional $\mathcal{L}$, after using the Gauss theorem, is

$$\begin{aligned} \delta I_t \;=\; & \int\limits_G \Big[(\boldsymbol{f} + \operatorname{Div}\mathbf{T} - \operatorname{Div}\operatorname{Div}\mathbf{M})\cdot\delta\boldsymbol{x} + (\mathsf{f} + \operatorname{Div}\mathbb{T}^{(2)})\cdot\delta\boldsymbol{X}\Big]\, dV - \\ & - \int\limits_{\partial G} \Big[\mathbb{T}^{(2)}\boldsymbol{N}\cdot\delta\boldsymbol{X} + (\mathbf{T} - 2\operatorname{Div}\mathbf{M})\boldsymbol{N}\cdot\delta\boldsymbol{x} + \mathbf{M}\boldsymbol{N}\cdot(\nabla\delta\boldsymbol{x} - \mathbf{F}\nabla\delta\boldsymbol{X})\Big]\, dS \end{aligned} \tag{3.9}$$

where

$$\mathbb{T}^{(2)} = \mathbb{T} + \mathbf{F}^\top \operatorname{Div}\mathbf{M} - (\nabla\mathbf{F})^\top\cdot\mathbf{M}$$

and the corresponding Euler-Lagrange equation for $\mathcal{L}$ is given by

$$\frac{\partial\mathcal{L}}{\partial\boldsymbol{x}} - \operatorname{Div}\frac{\partial\mathcal{L}}{\partial\mathbf{F}} + \operatorname{Div}\operatorname{Div}\frac{\partial\mathcal{L}}{\partial\nabla\mathbf{F}} = 0$$

Moreover, dS denotes the area element of the hypersurface ∂G bounding G, and $\boldsymbol{N} = ({}^x\boldsymbol{N}, {}^d\boldsymbol{N})$ is a suitably oriented unit vector normal to ∂G. The generalized divergence operators Div of $\mathbf{T} = ({}^x\mathbf{T}, {}^d\mathbf{T})$ and of $\mathbb{T} = ({}^x\mathbb{T}, {}^d\mathbb{T})$ are represented by

$$\begin{aligned} \operatorname{Div}{}^x\mathbf{T} &= {}^xD\,{}^x\mathbf{T} - \boldsymbol{N}_r\,{}^dD\,{}^x\mathbf{T} - {}^x\mathbf{T}\,{}^x\boldsymbol{\Gamma} \\ \operatorname{Div}{}^d\mathbf{T} &= {}^dD\,{}^d\mathbf{T} - {}^d\mathbf{T}\,{}^d\boldsymbol{\Gamma} \\ \operatorname{Div}{}^x\mathbb{T} &= -{}^x\nabla\mathcal{L} - {}^x\mathbf{F}^\top({}^x\boldsymbol{f} + \operatorname{Div}{}^x\mathbf{T}) \\ \operatorname{Div}{}^d\mathbb{T} &= -{}^d\nabla\mathcal{L} - ({}^d\mathbf{F})^\top({}^d\boldsymbol{f} + \operatorname{Div}{}^d\mathbf{T}) \end{aligned}$$

with the total differentials

$$\begin{aligned} {}^xD(\delta\boldsymbol{X}) &= {}^x\nabla(\delta\boldsymbol{X}) + \frac{\partial(\delta\boldsymbol{X})}{\partial^x\boldsymbol{\chi}_t}\,{}^x\nabla^x\boldsymbol{\chi}_t \\ {}^dD(\delta\boldsymbol{D}) &= {}^d\nabla(\delta\boldsymbol{D}) + \frac{\partial(\delta\boldsymbol{D})}{\partial^d\boldsymbol{\chi}_t}\,{}^d\nabla^d\boldsymbol{\chi}_t \end{aligned}$$

The representation for $\operatorname{Div}\mathbf{M}$ corresponds to $\operatorname{Div}\mathbf{T}$, the difference lies in the order of the tensors $\mathbf{M}$ and $\mathbf{T}$.

3.1. Correlation with the first-order variational formulation

Our starting point will be the functional

$$\begin{aligned} \delta I_t &= \int\limits_G \Big[(\boldsymbol{f} + \operatorname{Div}\mathbf{T} - \operatorname{Div}\operatorname{Div}\mathbf{M})\cdot\delta\boldsymbol{x} + (\mathfrak{f} + \operatorname{Div}\mathbb{T}^{(2)})\cdot\delta\boldsymbol{X}\Big]\, dV - \\ &- \int\limits_{\partial G} \Big[\mathbb{T}^{(2)}\boldsymbol{N}\cdot\delta\boldsymbol{X} + (\mathbf{T} - 2\operatorname{Div}\mathbf{M})\boldsymbol{N}\cdot\delta\boldsymbol{x}\Big]\, dS \end{aligned} \tag{3.10}$$

obtained from (3.9) by omitting the term $\mathbf{M}\boldsymbol{N}\cdot(\nabla\delta\boldsymbol{x} - \mathbf{F}\nabla\delta\boldsymbol{X})$ in the surface integral.

First, we adopt some notations for the stress and/or moment tensors valid for the second (and also higher) order variational formulation. Denote by $\mathbb{T}^{(n)} = ({}^x\mathbb{T}^{(n)}, {}^d\mathbb{T}^{(n)})$ the Eshelbian stress tensors for the nth order functional $\mathcal{L}$. In the same manner one can, if necessary, denote the stress tensor $\mathbf{T}$ by $\mathbf{T}^{(1)}$ and its higher order one by $\mathbf{T}^{(n)}$.

With this notation scheme our earlier Eshelbian stress tensor $\mathbb{T}$ will be identified by $\mathbb{T}^{(1)}$. The second order one, denoted by $\mathbb{T}^{(2)}$, is represented by

$$\begin{aligned} \mathbb{T}^{(2)} &= -\mathcal{L}\mathbf{I} - \mathbf{F}^\top\mathbf{T} + \mathbf{F}^\top\operatorname{Div}\mathbf{M} - (\nabla\mathbf{F})^\top\cdot\mathbf{M} = \\ &= \mathbb{T} + \mathbf{F}^\top\operatorname{Div}\mathbf{M} - (\nabla\mathbf{F})^\top\cdot\mathbf{M} \end{aligned} \tag{3.11}$$

where $\mathbf{I} = {}^x\mathbf{I} \oplus {}^d\mathbf{I}$.

Consider now a new first Piola-Kirchhoff type macro-micro stress tensor $\mathbf{T}^{(2)}$ defined as

$$\mathbf{T}^{(2)} = \mathbf{T} - \operatorname{Div}\mathbf{M} \tag{3.12}$$

which can be also obtained directly using the Volterra derivative (cf. Beris and Edwards, 1994)

$$\mathbf{T}^{(2)} = -\frac{\delta\mathcal{L}}{\delta\mathbf{F}} = -\frac{\partial\mathcal{L}}{\partial\mathbf{F}} + \operatorname{Div}\Big(\frac{\partial\mathcal{L}}{\partial\nabla\mathbf{F}}\Big)$$

In terms of $\mathbf{T}^{(2)}$, the equality (3.10) takes the simple form

$$\begin{aligned} \delta I_t &= \int\limits_G \Big[(\boldsymbol{f} + \operatorname{Div}\mathbf{T}^{(2)})\cdot\delta\boldsymbol{x} + (\mathfrak{f} + \operatorname{Div}\mathbb{T}^{(2)})\cdot\delta\boldsymbol{X}\Big]\, dV - \\ &- \int\limits_{\partial G} \Big[\mathbb{T}^{(2)}\boldsymbol{N}\cdot\delta\boldsymbol{X} + (\mathbf{T}^{(2)} - \operatorname{Div}\mathbf{M})\boldsymbol{N}\cdot\delta\boldsymbol{x}\Big]\, dS \end{aligned} \tag{3.13}$$

We close this paragraph with some remarks concerning different definitions of the stress tensors. Definitions (3.4) and (3.12), per se, suggest that T is a function of F, while $\mathsf{T}^{(2)}$ is addtionally gradient-dependent. The definition of $\mathsf{T}^{(2)}$ incorporates the first order gradient of F or the second order gradient in displacements. Formally, these two definitions are the same under the obvious identification of the first order variational formulation (Stumpf and Saczuk, 2000) with (3.10) and $\mathbb{T}$ with $\mathbb{T}^{(2)}$. Finally, there is no basic reason for limiting the consideration of the balance laws, at least for the mechanical part of the phenomenon discussed, to the first order case.

The balance laws and boundary conditions

The balance laws and boundary conditions for deformational and configurational forces resulting from the variational functional (3.13) are the following

(a) The balance of the deformational and configurational macro-micro momenta

$$\boldsymbol{f} + \mathrm{Div}\,\mathsf{T}^{(2)} = \mathbf{0} \qquad \mathfrak{f} + \mathrm{Div}\,\mathbb{T}^{(2)} = \mathbf{0} \tag{3.14}$$

where $\mathsf{T}^{(2)}$ is the first Piola-Kirchhoff macro-micro stress tensor, $\mathbb{T}^{(2)}$ the Eshelbian macro-micro stress tensor, $\boldsymbol{f}$ the external body macro-micro force, and $\mathfrak{f}$ the material inhomogeneity macro-micro force.

(b) The balance of moments of the deformational and configurational macro-micro momenta

$$\mathsf{T}^{(2)}\mathsf{F}^{\top} = \mathsf{F}(\mathsf{T}^{(2)})^{\top} \qquad \mathbb{T}^{(2)}\mathsf{C} = \mathsf{C}(\mathbb{T}^{(2)})^{\top} \tag{3.15}$$

where $\mathsf{C} = \mathsf{F}^{\top}\mathsf{F}$.

(c) The deformational and configurational macro-micro traction boundary conditions

$$(\mathsf{T}^{(2)} - \mathrm{Div}\,\mathsf{M})\boldsymbol{N} = \boldsymbol{t} \qquad \mathbb{T}^{(2)}\boldsymbol{N} = \mathbf{t} \tag{3.16}$$

where $\boldsymbol{t}$ and $\mathbf{t}$ are prescribed deformational and configurational boundary macro-micro tractions, respectively, and $\boldsymbol{N}$ is the outer vector normal to the boundary $\partial\mathfrak{B}$ in the actual and reference configuration, respectively.

3.2. Recourse to Mindlin's approach

We now study the first-order variation of I_t for an arbitrary variation of the placement in the actual and reference configurations

$$\begin{aligned}\delta I_t &= \int\limits_G \Big[(\boldsymbol{f} + \operatorname{Div}\mathbf{T}^{(2)})\cdot\delta\boldsymbol{x} + (\mathfrak{f} + \operatorname{Div}\mathbb{T}^{(2)})\cdot\delta\boldsymbol{X}\Big]\, dV - \\ &- \int\limits_{\partial G}\Big[\mathbb{T}^{(2)}\boldsymbol{N}\cdot\delta\boldsymbol{X} + (\mathbf{T}^{(2)} - \operatorname{Div}\mathbf{M})\boldsymbol{N}\cdot\delta\boldsymbol{x} + \mathbf{M}\boldsymbol{N}\cdot(\nabla\delta\boldsymbol{x} - \mathbf{F}\nabla\delta\boldsymbol{X})\Big]\, dS\end{aligned} \tag{3.17}$$

The given virtual displacement $\delta\boldsymbol{x}$ (on part) of ∂G can be used to determine its gradient on ∂G. Making use of this fact, one can eliminate the dependence of variation (3.17) on $\nabla\delta\boldsymbol{x} - \mathbf{F}\nabla\delta\boldsymbol{X}$. Based on Mindlin's approach (1965) (cf. Leroy and Molinari, 1993) we decompose the gradient $\nabla\delta\boldsymbol{x} - \mathbf{F}\nabla\delta\boldsymbol{X}$ into normal and surface terms

$$\nabla\delta\boldsymbol{x} - \mathbf{F}\nabla\delta\boldsymbol{X} = \overline{\nabla}\delta\boldsymbol{x} + \boldsymbol{N}\otimes\boldsymbol{N}\nabla\delta\boldsymbol{x} - \mathbf{F}(\overline{\nabla}\delta\boldsymbol{X} + \boldsymbol{N}\otimes\boldsymbol{N}\nabla\delta\boldsymbol{X})$$

where $\overline{\nabla}$ is the surface version of the spatial operator ∇. With the surface divergence theorem (see Brand, 1947)

$$\int\limits_S \overline{\nabla}\cdot(\mathbf{A}\boldsymbol{v})\, dS = \int\limits_S (\overline{\nabla}\cdot\boldsymbol{N})\boldsymbol{N}\mathbf{A}\cdot\boldsymbol{v}\, dS + \oint_C \boldsymbol{N}_C\mathbf{A}\cdot\boldsymbol{v}\, dC$$

where S is a smooth, closed surface, with the boundary C, $\overline{\nabla}$ the surface operator, $\boldsymbol{N}$ the unit vector normal to the surface S, $\boldsymbol{N}_C$ the unit vector normal to C and tangent to S, $\mathbf{A}$ a second-rank tensor, and $\boldsymbol{v}$ a vector. After neglecting the line intergral, the surface integral in (3.17) is modified such that the final expression for (3.17) reads

$$\begin{aligned}\delta I_t &= \int\limits_G \Big[(\boldsymbol{f} + \operatorname{Div}\mathbf{T}^{(2)})\cdot\delta\boldsymbol{x} + (\mathfrak{f} + \operatorname{Div}\mathbb{T}^{(2)})\cdot\delta\boldsymbol{X}\Big]\, dV - \\ &- \int\limits_{\partial G}\Big\{[(\mathbf{T}^{(2)} - \operatorname{Div}\mathbf{M})\boldsymbol{N} + (\operatorname{Div}_S\boldsymbol{N})\boldsymbol{N}\mathbf{M}\boldsymbol{N} - \operatorname{Div}_S(\mathbf{M}\boldsymbol{N})]\cdot\delta\boldsymbol{x} + \\ &+ [\mathbb{T}^{(2)}\boldsymbol{N} - (\operatorname{Div}_S\boldsymbol{N})\boldsymbol{N}\mathbf{F}\mathbf{M}\boldsymbol{N} + \operatorname{Div}_S(\mathbf{F}\mathbf{M}\boldsymbol{N})]\cdot\delta\boldsymbol{X}\Big\}\, dS - \\ &- \int\limits_{\partial G}[\boldsymbol{N}\mathbf{M}\boldsymbol{N}\cdot\nabla\delta\boldsymbol{x}\boldsymbol{N} - \boldsymbol{N}\mathbf{F}\mathbf{M}\boldsymbol{N}\cdot\nabla\delta\boldsymbol{X}\boldsymbol{N}]\, dS\end{aligned} \tag{3.18}$$

where $\operatorname{Div}_S(\cdot) \equiv \overline{\nabla} \cdot (\cdot)$ stands for the surface divergence operator.

Looking at the structure of (3.18), one can postulate the following generalized principle of a virtual surface work, valid for any surface Σ of $\mathfrak{B}$

$$\delta I_t = -\int_{\Sigma} (\boldsymbol{t} \cdot \delta \boldsymbol{x} + \boldsymbol{t}_{\Sigma} \cdot \nabla \delta \boldsymbol{x} \boldsymbol{N} + \mathbf{t} \cdot \delta \boldsymbol{X} + \mathbf{t}_{\Sigma} \cdot \nabla \delta \boldsymbol{X} \boldsymbol{N})\, dS \tag{3.19}$$

in which $\boldsymbol{t}$, $\boldsymbol{t}_{\Sigma}$ and $\mathbf{t}$, $\mathbf{t}_{\Sigma}$ are the deformational and configurational generalized tractions, respectively.

The corresponding equilibrium equations are the same as before, given by (3.14), but the deformational and configurational macro-micro traction boundary conditions take respectively the following forms

$$\begin{aligned} &(\mathbf{T}^{(2)} - \operatorname{Div} \mathbf{M})\boldsymbol{N} + (\operatorname{Div}_S \boldsymbol{N})\boldsymbol{N}\mathbf{M}\boldsymbol{N} - \operatorname{Div}_S(\mathbf{M}\boldsymbol{N}) = \boldsymbol{t} \\ &\boldsymbol{N}\mathbf{M}\boldsymbol{N} = \boldsymbol{t}_{\Sigma} \end{aligned} \tag{3.20}$$

and

$$\begin{aligned} &\mathbb{T}^{(2)}\boldsymbol{N} - (\operatorname{Div}_S \boldsymbol{N})\boldsymbol{N}\mathbf{F}\mathbf{M}\boldsymbol{N} + \operatorname{Div}_S(\mathbf{F}\mathbf{M}\boldsymbol{N}) = \mathbf{t} \\ &\boldsymbol{N}\mathbf{F}\mathbf{M}\boldsymbol{N} = \mathbf{t}_{\Sigma} \end{aligned} \tag{3.21}$$

where $\boldsymbol{N}$ is the outer vector normal to the boundary $\partial\mathfrak{B}$ in the actual and reference configuration.

3.2.1. Transversality conditions

The transversality conditions establish, in problems with movable boundaries like e.g. those connected with the evolution of crack surfaces, relations between the deformation gradient $\mathbf{F}$ and the gradients of macro- and microsurfaces in motion. In reality, they impose additional conditions on $\mathcal{L}$ necessary for an extremum of the action integral I_t. The extremum of I_t can only be obtained when the solution curve is one of the integral curves of the Euler-Lagrange equations (3.14) and (3.15).

The necessary conditions for an extremum $\delta I_t = 0$ according to (3.10) lead to

$$\mathbb{T}^{(2)}\boldsymbol{N} \cdot \delta \boldsymbol{X} + (\mathbf{T}^{(2)} - \operatorname{Div} \mathbf{M})\boldsymbol{N} \cdot \delta \boldsymbol{x} = 0 \qquad \text{on } \partial G \tag{3.22}$$

and, with respect to (3.18), to

$$\begin{aligned} &[(\mathbb{T}^{(2)} - \operatorname{Div} \mathbf{M})\boldsymbol{N} + (\operatorname{Div}_S \boldsymbol{N})\boldsymbol{N}\mathbf{M}\boldsymbol{N} - \operatorname{Div}_S(\mathbf{M}\boldsymbol{N})] \cdot \delta \boldsymbol{x} - \\ &-\boldsymbol{N}\mathbf{M}\boldsymbol{N} \cdot \nabla \delta \boldsymbol{x} \boldsymbol{N} + [\mathbb{T}^{(2)}\boldsymbol{N} - (\operatorname{Div}_S \boldsymbol{N})\boldsymbol{N}\mathbf{F}\mathbf{M}\boldsymbol{N} + \operatorname{Div}_S(\mathbf{F}\mathbf{M}\boldsymbol{N})] \cdot \delta \boldsymbol{X} - \\ &-\boldsymbol{N}\mathbf{F}\mathbf{M}\boldsymbol{N} \cdot \nabla \delta \boldsymbol{X} \boldsymbol{N} = 0 \qquad \text{on } \partial G \end{aligned} \tag{3.23}$$

These relations are of central importance in a number of nonlocal problems (e.g. Rice, 1968; Stumpf and Saczuk, 2001). If the variations $\delta\boldsymbol{X}$ and $\delta\boldsymbol{x}$ are independent, then

$$(\mathbf{T}^{(2)} - \operatorname{Div}\mathbf{M})\boldsymbol{N}\Big|_{P\in\Sigma} = \mathbf{0} \qquad \mathbb{T}^{(2)}\boldsymbol{N}\Big|_{P\in\Sigma} = \mathbb{O} \tag{3.24}$$

and

$$\begin{aligned}
&\Big[(\mathbb{T}^{(2)} - \operatorname{Div}\mathbf{M})\boldsymbol{N} + (\operatorname{Div}_S\boldsymbol{N})\boldsymbol{N}\mathbf{M}\boldsymbol{N} - \operatorname{Div}_S(\mathbf{M}\boldsymbol{N})\Big]_{P\in\Sigma} = \mathbf{0}\\
&\Big[\mathbb{T}^{(2)}\boldsymbol{N} - (\operatorname{Div}_S\boldsymbol{N})\boldsymbol{N}\mathbf{F}\mathbf{M}\boldsymbol{N} + \operatorname{Div}_S(\mathbf{F}\mathbf{M}\boldsymbol{N})\Big]_{P\in\Sigma} = \mathbb{O}
\end{aligned} \tag{3.25}$$

represent the homogeneous static boundary conditions of the Newtonian and Eshelbian type at any point P of the surface Σ, respectively.

3.3. Extension by including viscous contribution

If we assume $\boldsymbol{\alpha} = \{\boldsymbol{X}, \boldsymbol{D}, \boldsymbol{x}, \dot{\boldsymbol{x}}\}$ and $\boldsymbol{\beta} = \{\mathbf{F}, \nabla\mathbf{F}, \dot{\mathbf{F}}, \nabla\dot{\mathbf{F}}\}$ then the corresponding Euler-Lagrange equation for $\mathcal{L} = \mathcal{L}(\boldsymbol{\alpha}, \boldsymbol{\beta})$ is given by

$$\frac{\partial\mathcal{L}}{\partial\boldsymbol{x}} - \operatorname{Div}\frac{\partial\mathcal{L}}{\partial\mathbf{F}} - D_t\frac{\partial\mathcal{L}}{\partial\dot{\boldsymbol{x}}} + \operatorname{Div}\operatorname{Div}\frac{\partial\mathcal{L}}{\partial\nabla\mathbf{F}} + D_t\operatorname{Div}\frac{\partial\mathcal{L}}{\partial\dot{\mathbf{F}}} - D_t\operatorname{Div}\operatorname{Div}\frac{\partial\mathcal{L}}{\partial\nabla\dot{\mathbf{F}}} = 0 \tag{3.26}$$

with D_t denoting the material time derivative.

To obtain the continual version of the Euler-Lagrange equation, Eq. (3.26), we additionally adopt the following definitions

$$\boldsymbol{p} = \frac{\partial\mathcal{L}}{\partial\dot{\boldsymbol{x}}} \qquad \boldsymbol{\mathcal{P}} = \frac{\partial\mathcal{L}}{\partial\dot{\mathbf{F}}} \qquad \boldsymbol{\mathcal{M}} = \frac{\partial\mathcal{L}}{\partial\nabla\dot{\mathbf{F}}} \tag{3.27}$$

for the momenta of the zero-, first- and second-order, respectively. In this case Eq. (3.26) takes the form

$$D_t[\boldsymbol{p} - \operatorname{Div}(\boldsymbol{\mathcal{P}} - \operatorname{Div}\boldsymbol{\mathcal{M}})] = \boldsymbol{f} + \operatorname{Div}(\mathbf{T} - \operatorname{Div}\mathbf{M}) \tag{3.28}$$

the third-order equation of motion of the body $\mathfrak{B}$.

The stationarity conditions for the rate-dependent functional lead to the following equations of motion

$$\dot{\boldsymbol{p}} = \boldsymbol{f} + \operatorname{Div}(\mathbf{T}^{(2)} + \dot{\boldsymbol{\mathcal{P}}}^{(2)})$$

and

$$\dot{\mathfrak{p}} = \mathfrak{f} + \operatorname{Div}[\mathbb{T}^{(2)} + \mathbf{F}^{\top}\dot{\boldsymbol{\mathcal{P}}}^{(2)} + (\nabla\mathbf{F})^{\top}\cdot\dot{\boldsymbol{\mathcal{M}}}]$$

in the physical and material formulation, respectively. Finally, on the external or internal (movable) boundaries of the body, the boundary conditions take the following form

$$[\mathbb{T}^{(2)} + \mathsf{F}^{\top}\dot{\boldsymbol{\mathcal{P}}}^{(2)} + (\nabla\mathsf{F})^{\top} \cdot \dot{\boldsymbol{\mathcal{M}}}]\boldsymbol{N} \cdot \delta\boldsymbol{X} + [\mathsf{T}^{(2)} + \dot{\boldsymbol{\mathcal{P}}}^{(2)} - \operatorname{Div}(\mathsf{M} + \dot{\boldsymbol{\mathcal{M}}})]\boldsymbol{N} \cdot \delta\boldsymbol{x} = 0$$

where

$$\dot{\boldsymbol{\mathcal{P}}}^{(2)} = D_t(\boldsymbol{\mathcal{P}} - \operatorname{Div}\boldsymbol{\mathcal{M}}) \equiv \dot{\boldsymbol{\mathcal{P}}}^{(1)} - \operatorname{Div}\dot{\boldsymbol{\mathcal{M}}}$$

4. The dissipation inequality

In the non-thermal formulation, the second law of thermodynamics states that the rate of energy increase cannot exceed the total expended power. For the heat induced entropy flow, the second law is commonly written as the production entropy inequality

$$\frac{d}{dt}\int\limits_{B} \eta\, dV \geqslant -\int\limits_{\partial B} \theta^{-1}\boldsymbol{H} \cdot \boldsymbol{N}\, dS + \int\limits_{B} \theta^{-1}\dot{R}\, dV \tag{4.1}$$

where $\int_B \eta dV$ represents the internal entropy of B, the surface integral the entropy flow by heat conduction with the vector of heat flux $\boldsymbol{H}$, and the volume integral on the right hand side of inequality (4.1) the entropy flow by heat production $\dot{R}$ into B, neglected in the sequel. This inequality, known as the Clausius-Duhem inequality, is identified here with the sufficiency condition for functional (3.2) (cf. Stumpf and Saczuk, 2000).

The Euler-Lagrange equations (3.14), (3.15) and (3.16) or (3.22) of the Lagrangian (3.2) with arguments from Section 3.3 are not, in general, sufficient for the action integral I_t to attain an extreme value. The sufficiency conditions for I_t, strictly connected with the convexity conditions demanded by the dissipation inequality, can easily be obtained within the so-called method of equivalent integrals (Rund, 1966). This method, in principle, requires construction of a function Λ_t (a counterpart of the total derivative) and to form the integrand $\widetilde{\mathcal{L}}_t(\boldsymbol{X}, \boldsymbol{D}) = \mathcal{L}_t - \Lambda_t$ for a new action integral $\widetilde{I}_t(\boldsymbol{X}, \boldsymbol{D}) = \int_G \widetilde{\mathcal{L}}_t\, dV$ which, by definition, provides an extreme value to the same solutions as the solutions to the original problem defined by $I_t = \int_G \mathcal{L}_t\, dV$.

To solve this problem we have to consider the function Λ_t (Stumpf and Saczuk, 2000) and to define the Weierstrass excess function $\mathcal{E}$ as the difference

$$\mathcal{E} = \mathcal{L}_t(\widetilde{\boldsymbol{a}}; \widetilde{\boldsymbol{b}}) - \Lambda_t(\widetilde{\boldsymbol{a}}; \widetilde{\boldsymbol{b}}) \tag{4.2}$$

where $\widetilde{\boldsymbol{a}} = \{\widetilde{\theta}, \widetilde{\mathsf{F}}, \nabla\widetilde{\mathsf{F}}, \nabla\widetilde{\theta}\}$ and $\widetilde{\boldsymbol{b}} = \{\dot{\widetilde{\mathsf{F}}}, \nabla\dot{\widetilde{\mathsf{F}}}, \nabla\dot{\widetilde{\theta}}\}$. With these preliminary remarks the sufficiency condition of Weierstrass for a thermo-inelastic process of $\mathfrak{B}$ has the form

$$\mathcal{E} = \mathcal{E}(\boldsymbol{a}, \widetilde{\boldsymbol{a}}; \boldsymbol{b}, \widetilde{\boldsymbol{b}}) \geqslant 0 \tag{4.3}$$

valid for all $\widetilde{\mathsf{F}} = \mathsf{QF}$, $\nabla\widetilde{\mathsf{F}} = \mathsf{Q}\nabla\mathsf{F}$, etc. with arbitrary positive-definite tensor Q and for all constants ϑ such that $\widetilde{\theta} = \theta + \vartheta > 0$.

An explicit form of (4.3), accounting for inelastic and thermal effects, leads to a local Clausius-Duhem-type inequality in the physical form

$$\rho_0 \dot{\mathcal{L}}_t - (\mathsf{T}^{(2)} + \dot{\boldsymbol{\mathcal{P}}}^{(2)}) \cdot \dot{\mathsf{F}} + \theta^{-1} \nabla\theta \cdot \boldsymbol{H} \leqslant 0 \tag{4.4}$$

or, accounting additionally for the material (configurational) contributions in the form

$$\rho_0 \dot{\mathcal{L}}_t - (\mathsf{T}^{(2)} + \dot{\boldsymbol{\mathcal{P}}}^{(2)}) \cdot \dot{\mathsf{F}} - \overline{\mathbb{T}}^{(2)} \cdot \dot{\mathbb{F}} + \theta^{-1} \nabla\theta \cdot \boldsymbol{H} \leqslant 0 \tag{4.5}$$

where $\overline{\mathbb{T}}^{(2)} = \mathbb{T}^{(2)} + \mathsf{F}^\top \dot{\boldsymbol{\mathcal{P}}}^{(2)} + (\nabla\mathsf{F})^\top \cdot \dot{\boldsymbol{\mathcal{M}}}$, $\dot{\mathbb{F}}$ is a linear map of the configurational velocity, $\dot{\mathcal{L}}_t$ the rate of the energy functional per unit mass, ρ_0 the mass density in the reference configuration, θ the absolute temperature, and $\boldsymbol{H}$ the heat flux vector.

From the fact that the right-hand side of (4.5) never exceeds some finite upper bound, $\rho_0 \theta \dot{\eta}$ (Day, 1972) with η being the entropy, inequality (4.5) leads to the final form

$$\rho_0(\eta\dot{\theta} + \dot{\Psi}) - (\mathsf{T}^{(2)} + \dot{\boldsymbol{\mathcal{P}}}^{(2)}) \cdot \dot{\mathsf{F}} - \overline{\mathbb{T}}^{(2)} \cdot \dot{\mathbb{F}} + \theta^{-1} \nabla\theta \cdot \boldsymbol{H} \leqslant 0 \tag{4.6}$$

expressed in terms of the Helmholtz free energy $\Psi = \mathcal{L}_t - \theta\eta$ as a state variable. When this inequality holds with the equality sign, the thermodynamic process is called reversible, otherwise irreversible. This form of the entropy inequality is meaningful when the temperature is used as an independent thermal variable.

Because of the rate-dependency of η, $\mathsf{T}^{(2)}$, $\dot{\boldsymbol{\mathcal{P}}}^{(2)}$ and $\boldsymbol{H}$, it is necessary to find their changes (towards the equilibrium state) between any two times t_0 and t_1 on any path of the thermo-inelastic process for which inequality (4.6) holds. This can be only valid if the following differences (cf. Day, 1972)

$$\eta - \eta^\star, \quad \mathsf{T}^{(2)} - \mathsf{T}^\star, \quad \dot{\boldsymbol{\mathcal{P}}}^{(2)} - \boldsymbol{\mathcal{P}}^\star, \quad \overline{\mathbb{T}}^{(2)} - \overline{\mathbb{T}}^\star \quad \text{and} \quad \boldsymbol{H} - \boldsymbol{H}^\star$$

according to the non-vanishing rates $\dot{\mathsf{F}}$, $\dot{\mathbb{F}}$ and $\dot{\theta}$ satisfy inequality (4.6) on any thermo-inelastic path. The quantities with on asterisk refer to the corresponding values at the equilibrium.

The only thermodynamic information that we have now is the positive definiteness of the entropy production, which imposes some restrictions on the possible form of the evolution (relaxation) equations of thermodynamic fluxes. Within the formalism of extended irreversible thermodynamics, we have to generalize dissipation inequality (4.6) by including the relaxation terms for transport processes via the relaxation entropy concept η_r (Sieniutycz, 1981a,b). We assume also that the non-equilibrium entropy is only defined when the deviations from the equilibrium state are not too large. For thermo-inelastically deformed solids, for instance, the relaxation entropy takes the form

$$\eta_r(\mathbf{S}^\circ, \boldsymbol{H}) = \frac{1}{2G} C^{-1}[\boldsymbol{H}] \cdot \boldsymbol{H} - \frac{1}{4\theta G} \mathbf{S}^\circ \cdot \mathbf{S}^\circ \tag{4.7}$$

where by $\mathbf{S}^\circ$ we denote an objective deviatoric form of the stress tensor $\mathbf{T}^{(2)} + \dot{\mathcal{P}}^{(2)}$, C is the thermostatic capacity tensor and G the shear modulus. For example, in the case of pure heat diffusion we have $C := \partial h / \partial \nabla \theta^{-1}$, where h is the enthalpy.

Substituting

$$\mathbf{S} \cdot \dot{\mathbf{C}} = \mathbf{S}^\circ \cdot \dot{\mathbf{C}}^\circ + \frac{1}{3} \operatorname{tr} \mathbf{S} \operatorname{tr} \dot{\mathbf{C}} \tag{4.8}$$

and (4.7) into inequality (4.6), written in the objective form, we get

$$\begin{aligned} &\rho_0(\eta_t \dot{\theta} + \dot{\Psi}) - \mathbf{S}^\circ \cdot \dot{\mathbf{C}}^\circ - \frac{1}{3} \operatorname{tr} \mathbf{S} \operatorname{tr} \dot{\mathbf{C}} + \frac{1}{G} C^{-1}[\boldsymbol{H}] \cdot \dot{\boldsymbol{H}} - \frac{1}{2\theta G} \mathbf{S}^\circ \cdot \dot{\mathbf{S}}^\circ - \\ &- \overline{\mathbb{T}}^{(2)} \cdot \dot{\mathbb{F}} + \theta^{-1} \nabla \theta \cdot \boldsymbol{H} \leqslant 0 \end{aligned} \tag{4.9}$$

where

$$\eta_t(U, \mathbf{S}^\circ, \boldsymbol{H}) = \eta(U) + \eta_r(\mathbf{S}^\circ, \boldsymbol{H})$$

is the total entropy and $U = U(\mathbf{C}, \theta)$ the internal energy. In the above derivation we have assumed the shear modulus G to be time independent.

5. Constitutive equations

To complete the set of equations defining a thermodynamical theory of continuum mechanics we have to postulate appropriate constitutive equations for the specified class of materials. In the following we select as independent variables in the constitutive equations the macro- and microstrain tensors ${}^x\mathbf{E}$ and ${}^d\mathbf{E}$, the deformation-induced anisotropy tensor $\mathbf{A}_F$, the temperature θ and their rates to describe the thermomechanical behaviour of solids with a specific microstructure.

In the light of the axiom of equipresence, the arguments of the constitutive quantities η, ${}^x\mathsf{S}$, ${}^d\mathsf{S}$ and $\boldsymbol{H}$ may be selected as

$$\begin{aligned}
\eta &= \widehat{\eta}(\mathsf{E},\theta,\nabla\theta,\dot{\mathsf{E}},\dot{\theta},\mathsf{A}_F) \equiv \widehat{\eta}({}^x\mathsf{E},{}^d\mathsf{E},\theta,\nabla\theta,\dot{\mathsf{E}},{}^d\dot{\mathsf{E}},\dot{\theta},\mathsf{A}_F)\\
{}^x\mathsf{S} &= \widehat{\mathsf{S}}(\mathsf{E},\theta,\nabla\theta,\dot{\mathsf{E}},\dot{\theta},\mathsf{A}_F) \equiv {}^x\widehat{\mathsf{S}}({}^x\mathsf{E},{}^d\mathsf{E},\theta,\nabla\theta,\dot{\mathsf{E}},{}^d\dot{\mathsf{E}},\dot{\theta},\mathsf{A}_F)\\
{}^d\mathsf{S} &= {}^d\widehat{\mathsf{S}}(\mathsf{E},\theta,\nabla\theta,\dot{\mathsf{E}},\dot{\theta},\mathsf{A}_F) \equiv {}^d\widehat{\mathsf{S}}({}^x\mathsf{E},{}^d\mathsf{E},\theta,\nabla\theta,\dot{\mathsf{E}},{}^d\dot{\mathsf{E}},\dot{\theta},\mathsf{A}_F)\\
\boldsymbol{H} &= \widehat{\boldsymbol{H}}(\mathsf{E},\theta,\nabla\theta,\dot{\mathsf{E}},\dot{\theta},\mathsf{A}_F) \equiv \widehat{\boldsymbol{H}}({}^x\mathsf{E},{}^d\mathsf{E},\theta,\nabla\theta,\dot{\mathsf{E}},{}^d\dot{\mathsf{E}},\dot{\theta},\mathsf{A}_F)
\end{aligned} \tag{5.1}$$

in which the response functions $\widehat{\eta}$, ${}^x\widehat{\mathsf{S}}$, ${}^d\widehat{\mathsf{S}}$ and $\widehat{\boldsymbol{H}}$ for the entropy, macro- and microstress tensors and the heat flux vector are the characteristics of the material. The variables ${}^x\mathsf{E}$, ${}^d\mathsf{E}$, θ, ${}^x\dot{\mathsf{E}}$, ${}^d\dot{\mathsf{E}}$, $\dot{\theta}$ and A_F are, by definition, functions of the reference vectors $\boldsymbol{X}$, $\boldsymbol{D}$ and time t.

Case without relaxation

The first simplification consists in neglecting η_r. In this case inequality (4.9) is reduced to

$$\rho_0(\eta\dot{\theta}+\dot{\Psi}) - \mathsf{S}\cdot\dot{\mathsf{E}} + \theta^{-1}\nabla\theta\cdot\boldsymbol{H} \leqslant 0 \tag{5.2}$$

To specify a material, we assume that the generalized free energy functional $\widetilde{\Psi}$ depends only on the strain, the temperature and their rates as independent variables. It means that the generalized free energy $\widetilde{\Psi}$ can be written in the form

$$\widetilde{\Psi} = \widetilde{\Psi}(\mathsf{E},\theta,\dot{\mathsf{E}},\dot{\theta},\mathsf{A}_F) \equiv \widetilde{\Psi}({}^x\mathsf{E},{}^d\mathsf{E},\theta,{}^x\dot{\mathsf{E}},{}^d\dot{\mathsf{E}},\dot{\theta},\mathsf{A}_F)$$

Calculating the material time derivative of $\widetilde{\Psi}$ we get

$$\dot{\widetilde{\Psi}} = \frac{\delta\widetilde{\Psi}}{\delta^x\mathsf{E}}\cdot{}^x\dot{\mathsf{E}} + \frac{\partial\widetilde{\Psi}}{\partial^d\mathsf{E}}\cdot{}^d\dot{\mathsf{E}} + \frac{\partial\widetilde{\Psi}}{\partial\theta}\dot{\theta} + \frac{\delta\widetilde{\Psi}}{\delta^x\dot{\mathsf{E}}}\cdot{}^x\ddot{\mathsf{E}} \tag{5.3}$$

where the differential operators $\delta/\delta^x\mathsf{E}$ and $\delta/\delta\dot{\mathsf{E}}$ are defined by the relations

$$\frac{\delta}{\delta^x\mathsf{E}} = \frac{\partial}{\partial^x\mathsf{E}} - \boldsymbol{N}_F\frac{\partial}{\partial^d\mathsf{E}} \qquad\qquad \frac{\delta}{\delta\dot{\mathsf{E}}} = \frac{\partial}{\partial\dot{\mathsf{E}}} - \boldsymbol{N}_\theta\frac{\partial}{\partial\dot{\theta}}$$

The objects $\boldsymbol{N}_F$ and $\boldsymbol{N}_\theta$ represent material connections, first, correlated with the deformation-induced anisotropy tensor A_F, second, with the thermo-mechanical coupling (Boffi et al., 1980). In this case the connection $\boldsymbol{N}_F$ should be expressed by E, while $\boldsymbol{N}_\theta$, according to Boffi et al. (1980), can be approximated by

$$\boldsymbol{N}_\theta = -\theta_0\boldsymbol{\gamma} + \frac{2\mu}{C_V}\,{}^x\dot{\mathsf{E}}$$

where ${}^x\boldsymbol{\gamma}_G$ is the Grüneisen (thermomechanical coupling) tensor, μ the viscosity coefficient, C_V the specific heat at constant volume and θ_0 the reference temperature.

In terms of Eq. (5.3) inequality (5.2) gives rise to

$$\begin{aligned}&\rho\Big(\eta+\frac{\partial\widetilde{\Psi}}{\partial\theta}\Big)\cdot\dot{\theta}+\Big(\rho_0\frac{\delta\widetilde{\Psi}}{\delta^x\mathsf{E}}-{}^x\mathsf{S}\Big)\cdot{}^x\dot{\mathsf{E}}+\Big(\rho_0\frac{\partial\widetilde{\Psi}}{\partial^d\mathsf{E}}-{}^d\mathsf{S}\Big)\cdot{}^d\dot{\mathsf{E}}+\\&+\rho_0\frac{\delta\widetilde{\Psi}}{\delta^x\dot{\mathsf{E}}}\cdot{}^x\ddot{\mathsf{E}}+\nabla\ln\theta\cdot\boldsymbol{H}\leqslant 0\end{aligned}\tag{5.4}$$

This inequality can hold for all choices of ${}^x\ddot{\mathsf{E}}$ only if

$$\frac{\delta\widetilde{\Psi}}{\delta^x\dot{\mathsf{E}}}\equiv\frac{\partial\widetilde{\Psi}}{\partial^x\dot{\mathsf{E}}}-\boldsymbol{N}_\theta\frac{\partial\widetilde{\Psi}}{\partial\dot{\theta}}=0$$

This constraint means that the generalized free energy is dependent on the rate $\dot{\theta}$ via the rate ${}^x\dot{\mathsf{E}}$. Therefore, the generalized stresses are determined by the response function $\widetilde{\Psi}=\widetilde{\Psi}(\mathsf{E},\theta,\dot{\mathsf{E}}(\dot{\theta}))$ and in the equlibrium by $\widetilde{\Psi}^\star(\mathsf{E},\theta)=\widetilde{\Psi}(\mathsf{E},\theta,\mathbf{0})$.

In the same manner, from the requirement that inequality (5.4) is fulfilled for all choices of $\dot{\theta},{}^x\dot{\mathsf{E}}$ and ${}^d\dot{\mathsf{E}}$, we get

$$\eta=-\frac{\partial\widetilde{\Psi}}{\partial\theta}\qquad {}^x\mathsf{S}=\rho_0\Big(\frac{\partial\widetilde{\Psi}}{\partial^x\mathsf{E}}-\boldsymbol{N}_F\frac{\partial\widetilde{\Psi}}{\partial^d\mathsf{E}}\Big)\qquad {}^d\mathsf{S}=\rho_0\frac{\partial\widetilde{\Psi}}{\partial^d\mathsf{E}}\tag{5.5}$$

as the necessary constitutive relations.

As a simple illustration for the discussed problem, let us consider the free energy functional Ψ defined only in terms of the strain measures ${}^x\mathsf{E}$ and ${}^d\mathsf{E}$. Applying Eqs (5.5) to Ψ we get

$${}^x\mathsf{S}=\rho_0\Big(\frac{\partial\Psi}{\partial^x\mathsf{E}}-\boldsymbol{N}_F\frac{\partial\Psi}{\partial^d\mathsf{E}}\Big)\qquad {}^d\mathsf{S}=\rho_0\frac{\partial\Psi}{\partial^d\mathsf{E}}\tag{5.6}$$

To show the correlation with classical results, it is enough to adopt an obvious functional relation between E and ${}^x\mathsf{E}$, where the classical strain measure E is defined in terms of the deformation gradient $\mathsf{F}=\partial\boldsymbol{x}/\partial\boldsymbol{X}$. Based on (5.6) we obtain with

$$\mathsf{S}=\rho_0\frac{\partial\Psi}{\partial\mathsf{E}}=\rho_0\frac{\partial\Psi}{\partial^x\mathsf{E}}\,\frac{\partial^x\mathsf{E}}{\partial\mathsf{E}}=({}^x\mathsf{S}+\boldsymbol{N}_F{}^d\mathsf{S})\mathbb{A}_E\qquad \mathbb{A}_E=\frac{\partial^x\mathsf{E}}{\partial\mathsf{E}}\tag{5.7}$$

a functional relation between the classical stress tensor S and the macrostress tensor ${}^x\mathsf{S}$ derived in the anlysis presented here. The equality $\mathsf{S}={}^x\mathsf{S}$ can only be obtained if the reference anisotropy tensor $\mathbf{A}_r$ reduces to the identity tensor (or $\mathbb{A}_E \equiv \mathbb{I}$) and, at the same time, the deformation-induced anisotropy tensor $\mathbf{A}_F$ is singular at each step of the deformation process. Furthermore, any detail connected with the internal state has to be neglected.

Case with relaxation

The entropy production terms

$$\sigma_{\boldsymbol{H}} \equiv \frac{1}{\theta G} C^{-1}[\boldsymbol{H}] \cdot \dot{\boldsymbol{H}} + \nabla\theta^{-1} \cdot \boldsymbol{H}$$

in inequality (4.9) on the basis of Curie's principle is equal to

$$\boldsymbol{H} = \boldsymbol{L}_{\boldsymbol{H}} \Big(\frac{1}{G} C^{-1}[\dot{\boldsymbol{H}}] + \nabla\theta^{-1} \Big) \tag{5.8}$$

where $\boldsymbol{L}_{\boldsymbol{H}}$ is the positive definite Onsager tensor. For the case of pure heat diffusion, $\boldsymbol{L}_{\boldsymbol{H}} = \boldsymbol{\lambda}\theta^2$, where $\boldsymbol{\lambda}$ is the conductivity coefficient tensor. In this case Eq. (5.8) can be replaced by the equation

$$\boldsymbol{H} + \tau\dot{\boldsymbol{H}} = -\boldsymbol{\lambda}\nabla\theta$$

As a result, the above evolution equation for the heat flux vector $\boldsymbol{H}$ is compatible with the Cattaneo equation for pure heat diffusion (Cattaneo, 1948), $\boldsymbol{q} + \tau\dot{\boldsymbol{q}} = -\lambda\nabla\theta$, where τ is the relaxation time of the heat flux vector $\boldsymbol{q}$.

Application of the same procedure to the term

$$\sigma_{\boldsymbol{S}} \equiv -\frac{1}{\theta} \Big(\mathbf{S}^\circ \cdot \dot{\mathbf{E}}^\circ + \frac{1}{2G} \mathbf{S}^\circ \cdot \dot{\mathbf{S}}^\circ \Big)$$

in inequality (4.9) gives rise to the following evolution equation for $\mathbf{S}^\circ$

$$\mathbf{S}^\circ + \frac{\mu_d}{G} \dot{\mathbf{S}}^\circ = -\mu_d \dot{\mathbf{E}}^\circ$$

which is known as the Maxwell equation for momentum diffusion in a viscous (in)elastic body. In this case an appropriate Onsager tensor is defined by the symmetry relation, $\boldsymbol{L}_{\boldsymbol{S}} = 2\mu_d\theta$, with μ_d being the dynamic viscosity coefficient.

6. Application: A solid-void continuum model

In this section we sketch a solid-void continuum model to describe the inelastic process in solids. To be in agreement with the solid-solid phase modelling (Pagano et al., 1998) we assume that the thermomechanical aspects of an inelastic process are completely determined by the free energy of a solid-void continuum (a body with defects), denoted by Ψ, and by the dissipation functional Φ (collectively denoted by $\mathcal{L}_t$ as a function of Ψ and Φ).

As an example, let us consider (cf. Pagano and Alart, 1999)

$$\Psi(\mathbf{E}, \mathbf{E}_d, \Omega, \theta) = (1 - \Omega)\Psi_c(\mathbf{E}, \theta) + \Omega\Psi_d(\mathbf{E}_d, \theta) + \Psi_{int}(\Omega, \theta)$$

where Ω is the volume fraction of voids in the body, Ψ_c the free energy of the body without defects, Ψ_d the free energy of the damage phase, Ψ_{int} the interaction energy between the solid-void phases, and $\mathbf{E}_d$ the defect measure. By assumption, $\Psi(\cdot, \Omega, \theta)$ has multiple local energy minima corresponding to the solid and void phases. For our purpose we choose

$$\rho_0\Psi_c(\mathbf{E}, \theta) = \frac{1}{2}\mathbb{C}_c[\mathbf{E}] \cdot \mathbf{E} - C_V(\theta - \theta_c)\boldsymbol{\gamma} \cdot (\mathbf{E} + \mathbf{E}_d) - \frac{C_V}{\theta_c}\rho_0(\theta - \theta_c)^2$$

$$\rho_0\Psi_d(\mathbf{E}_d, \theta) = \frac{1}{2}\mathbb{C}_d[\mathbf{E}_d] \cdot \mathbf{E}_d + C_V(\theta - \theta_c)\boldsymbol{\gamma}_d \cdot (\mathbf{E} + \mathbf{E}_d) - \frac{C_V}{\theta_c}\rho_0(\theta - \theta_c)^2$$

$$\Psi_{int}(\Omega, \theta) = \frac{C(\theta)}{2}[\Omega - \Omega^2] + M(\Omega)$$

where $\boldsymbol{\gamma}$ and $\boldsymbol{\gamma}_d$ are the Grüneisen tensors defined by (cf. Stumpf and Saczuk, 2000)

$$\boldsymbol{\gamma} = \rho_0\Big(\theta\frac{\partial^2\Psi_c}{\partial\theta^2}\Big)^{-1}\frac{\partial^2\Psi_c}{\partial\theta\partial\mathbf{E}} \qquad\qquad \boldsymbol{\gamma}_d = \rho_0\Big(\theta\frac{\partial^2\Psi_d}{\partial\theta^2}\Big)^{-1}\frac{\partial^2\Psi_d}{\partial\theta\partial\mathbf{E}_d}$$

θ_c is the characteristic temperature of the material, C_V the specific heat at constant volume and $C(\theta)$, $M(\Omega)$ known material functions.

The form of the interaction energy Ψ_{int} can be used to define the convexity or non-convexity of the potential, and thus the stability or instability of the material behaviour. In general, we expect that Ω minimizes the solid-void phase energy Ψ_{int}.

It is assumed that the state variables $(\mathbf{E}, \mathbf{E}_d, \Omega, \theta)$ obey the following constitutive laws

$$\mathbf{S}_e = \frac{\partial\Psi}{\partial\mathbf{E}} \qquad \mathbf{S}_{de} = \frac{\partial\Psi}{\partial\mathbf{E}_d} \qquad A \in \partial_\Omega\Psi \qquad \eta = -\frac{\partial\Psi}{\partial\theta} \tag{6.1}$$

where A is the thermodynamic function associated with the fraction Ω.

Dissipation inequality (4.4) suggests assuming a dissipation potential Φ as a function of $\dot{\mathbf{E}}$, $\dot{\mathbf{E}}_d$ and $\dot{\Omega}$. In terms of Φ one can write then the constitutive laws, see Eqs (6.1), in the complementary form

$$\mathbf{S}_v = \frac{\partial \Phi}{\partial \dot{\mathbf{E}}} \qquad \mathbf{S}_{dv} = \frac{\partial \Phi}{\partial \dot{\mathbf{E}}_d} \qquad A = -\frac{\partial \Phi}{\partial \dot{\Omega}}$$

where $\mathbf{S}_v$ and $\mathbf{S}_{dv}$ are the irreversible parts of the stress tensors $\mathbf{S}$ and $\mathbf{S}_d$.

7. Conclusion

In this paper a nonlocal gradient model of inelastic heterogeneous media is presented, which can be considered as a framework general enough to account for mechanisms in a material with different lengthscales by using a 6-dimensional non-Euclidean manifold structure and including strain gradient terms. This enables derivation of various nonlocal and gradient, theories by introducing simplifying assumptions. Balance laws for physical and configurational forces on a macro- and microlevel are derived and boundary and transversality conditions are given. The dissipation inequality and the constitutive modelling are discussed taking into account also relaxation processes. As an application a solid-void continuum model is considered.

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Nielokalny model gradientowy niesprężystych ośrodków heterogenicznych

Streszczenie

Celem pracy jest zbadanie wpływu nielokalności na fizyczne i materialne równania pola ośrodków heterogenicznych. Biorąc pod uwagę, że plastyczna deformacja w metalach lub zniszczenie w kruchych i ciągliwych materiałach rządzone są przez fizyczne mechanizmy na różnych poziomach skali, wprowadzono 6-wymiarową strukturę z dwoma lokalnie zdefiniowanymi wektorami do modelowania materialnego zachowania ośrodka na poziomie makro- i mezo- lub mikroskali.

Wykorzystując wariacyjną procedurę otrzymano fizyczne i materialne prawa bilansu, warunki brzegowe i transwersalności dla makro- i mikrodeformacji ośrodków heterogenicznych. Przedstawiona nierówność dyssypacyjna zawiera człony relaksacyjne

procesów transportu. Sformułowane równania konstytutywne wyrażono przy pomocy miar makro- i mikroodkształcenia, ich gradientów i przyrostów oraz tensora anizotropii, gdzie ostatni argument może być traktowany jako miara sprzężenia pomiędzy odkształconymi makrostanami i kompatybilnymi mikrostanami.

Przedstawiony w pracy model dostarcza podstaw, które poprzez wprowadzenie uproszczających założeń umożliwiają otrzymanie różnych postaci nielokalnych i gradientowych teorii. Jako przypadek szczególny rozpatrzono model typu ciało stałe-pustka.

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